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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	AUG 10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS 3	AUG 18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS 4	AUG 24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS 5	AUG 24	CA/CAplus enhanced with legal status information for U.S. patents
NEWS 6	SEP 09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS 7	SEP 11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus
NEWS 8	OCT 21	Derwent World Patents Index Coverage of Indian and Taiwanese Content Expanded
NEWS 9	OCT 21	Derwent World Patents Index enhanced with human translated claims for Chinese Applications and Utility Models
NEWS 10	OCT 27	Free display of legal status information in CA/CAplus, USPATFULL, and USPAT2 in the month of November.

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

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Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 11:21:10 ON 03 NOV 2009

=> fil reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION

FULL ESTIMATED COST 0.22 0.22

FILE 'REGISTRY' ENTERED AT 11:21:24 ON 03 NOV 2009

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 NOV 2009 HIGHEST RN 1190833-66-9
DICTIONARY FILE UPDATES: 1 NOV 2009 HIGHEST RN 1190833-66-9

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TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
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L1 STRUCTURE UPLOADED

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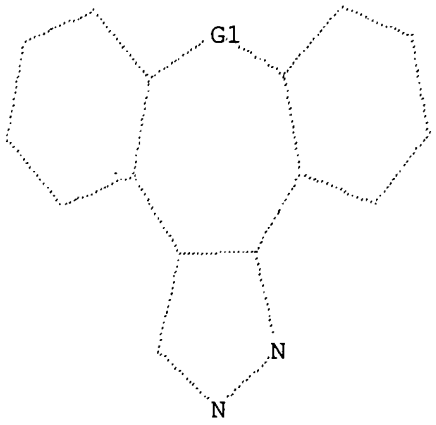
L1 HAS NO ANSWERS
L1 STR



G1 C,S,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full
FULL SEARCH INITIATED 11:22:02 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 14441 TO ITERATE

100.0% PROCESSED 14441 ITERATIONS 94 ANSWERS
SEARCH TIME: 00.00.01

L2 94 SEA SSS FUL L1

=> fil hcap
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	185.88	186.10

FILE 'HCAPLUS' ENTERED AT 11:22:08 ON 03 NOV 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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FILE COVERS 1907 - 3 Nov 2009 VOL 151 ISS 19
FILE LAST UPDATED: 2 Nov 2009 (20091102/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Aug 2009
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

http://www.cas.org/legal/infopolicy.html

This file contains CAS Registry Numbers for easy and accurate substance identification.

During November, try the new LSUS format of legal status information in the CA/CAplus family databases for free! Complete details on the number of free displays and other databases participating in this offer appear in NEWS 10.

=> l2
L3 16 L2

=> l3 and neurotransmitter
50218 NEUROTRANSMITTER
27509 NEUROTRANSMITTERS
62651 NEUROTRANSMITTER
(NEUROTRANSMITTER OR NEUROTRANSMITTERS)
L4 1 L3 AND NEUROTRANSMITTER

=> l3 and CNS

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         46425 CNS
             1 CNSES
         46426 CNS
                 (CNS OR CNSES)
L5           1 L3 AND CNS

=> d l3 ibib abs hitstr 1-16
```

L3 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

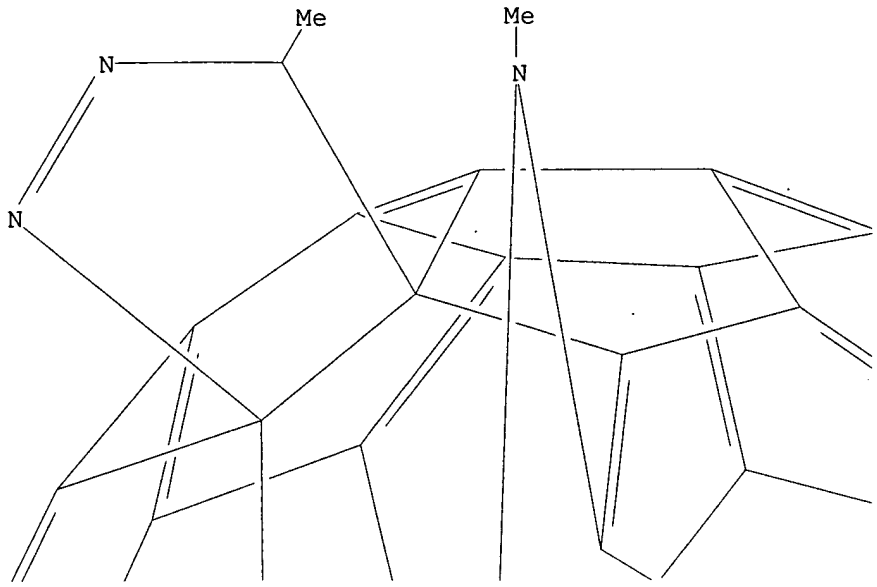
ACCESSION NUMBER: 2006:595313 HCAPLUS
DOCUMENT NUMBER: 145:396897
TITLE: Theoretical study on the reaction mechanism of bis-addition of methyl azide to C60 (II)
AUTHOR(S): Zhuang, Xuxia; Yang, Zuoyin; Zhang, Jingchang; Cao, Weiliang
CORPORATE SOURCE: State Key Laboratory of Chemical Resource Engineering, Faculty of Science, Beijing University of Chemical Technology, Beijing, 100029, Peop. Rep. China
SOURCE: THEOCHEM (2006), 765(1-3), 53-59
CODEN: THEODJ; ISSN: 0166-1280
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The processes of 1,3-dipolar cycloaddn. (1,3-DC) of Me azide to azafulleroid (C60NCH3) were studied by using AM1 semi-empirical and d. functional methods. Based on the charge distributions of the reagents, there are four most possible modes for Me azide to attack the double bonds of C60NCH3. In each case, N2 extrusion takes place via two steps, which is consequent upon the formation of a triazoline intermediate. The first step is the breaking of a N-N single bond, and the second one undergoes the liberation of a N2 mol. with the simultaneous formation of a new C-N bond. Three bisazafulleroid isomers would be produced through the four reaction paths, one of which has two N atoms bonded to two neighboring open 5-6 junctions of the same pentagon, and the other two have their N atoms bonded to the alternate open 5-6 junctions around the same pentagon and the same hexagon, resp. Because of the interlacements of their corresponding energy barriers in the rate-controlling steps, interaction energies and the apparent active energies, the four reaction modes will all possibly occur in principle.

IT **911482-51-4**
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(mechanistic reaction intermediate; theor. study on reaction mechanism of bis-addition of Me azide to C60)

RN 911482-51-4 HCAPLUS
CN 5'H-2a-Aza-1,2(2a)-homo[5,6]fullereno-C60-Ih-[11,10-c]pyrazole, 2a,5'-dimethyl- (9CI) (CA INDEX NAME)

PAGE 1-A



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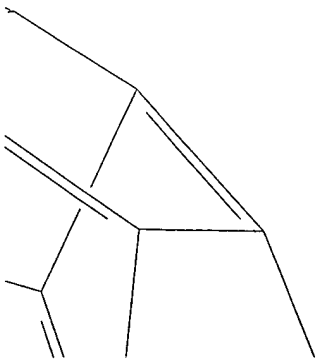

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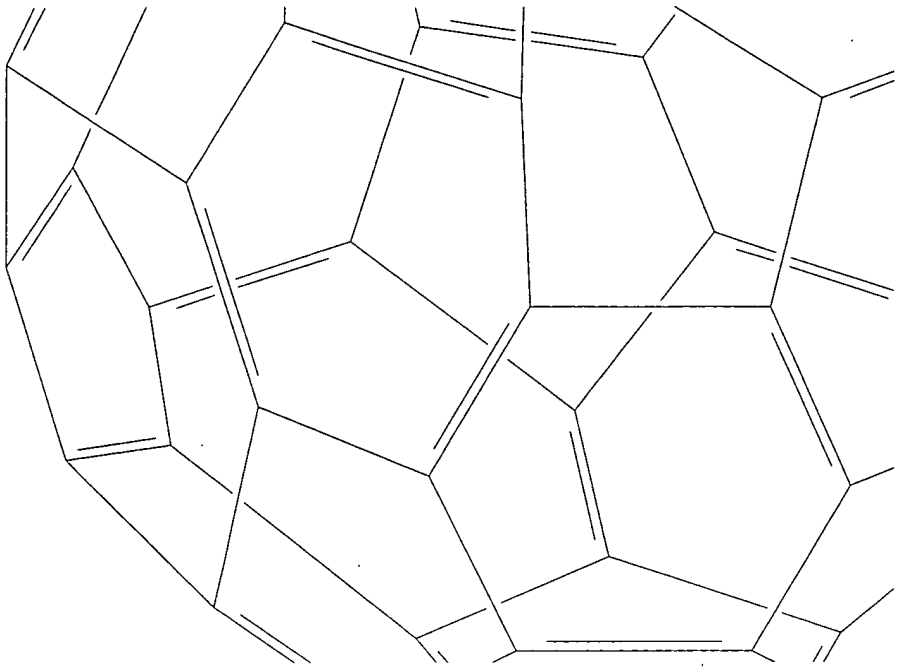

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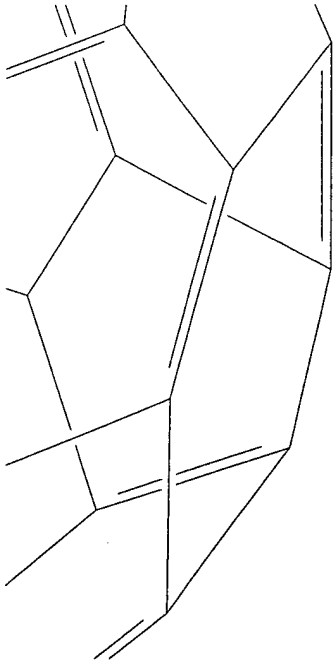
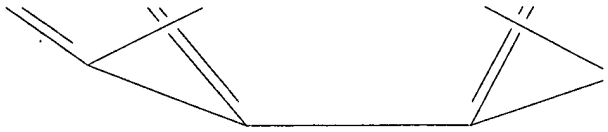


PAGE 3-A



PAGE 3-B

OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:471942 HCAPLUS
DOCUMENT NUMBER: 143:13341
TITLE: 1,2-Diazadibenzo[e,h]azulene pharmaceuticals for the treatment of central nervous system diseases
INVENTOR(S): Mercep, Mladen; Mesic, Milan; Pesic, Dijana
PATENT ASSIGNEE(S): Pliva-Istrazivacki Institut D.O.O., Croatia
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005049015	A1	20050602	WO 2004-HR53	20041119
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2546590	A1	20050602	CA 2004-2546590	20041119
EP 1686989	A1	20060809	EP 2004-798732	20041119
EP 1686989	B1	20090114		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU				
CN 1901904	A	20070124	CN 2004-80038551	20041119
JP 2007512307	T	20070517	JP 2006-540630	20041119
AT 420637	T	20090115	AT 2004-798732	20041119
ES 2320229	T3	20090520	ES 2004-798732	20041119

IN 2006CN02230	A	20070608	IN 2006-CN2230		20060621
US 20070173492	A1	20070726	US 2006-595934		20060811
PRIORITY APPLN. INFO.:			HR 2003-956	A	20031121
			WO 2004-HR53	W	20041119

OTHER SOURCE(S): MARPAT 143:13341

AB The present invention relates to the use of compds. from the group of 1,2-diazadibenzo[e,h]azulenes and of their salts and solvates for the manufacture of a pharmaceutical formulation for the treatment of diseases, damages and disorders of the central nervous system (CNS) caused by disorders of the neurochem. equilibrium of biogenic amines or other neurotransmitters. Thus, a diazadibenzo[e,h]azulene reduced the CNS disorder induced by m-CPP.

IT **629653-99-2** **629654-01-9** **629654-03-1**
629654-05-3 **629654-09-7** **629654-10-0**
629654-11-1 **629654-12-2** **629654-15-5**
629654-16-6 **629654-23-5** **629654-24-6**
629654-25-7 **629654-26-8** **629654-27-9**
629654-28-0
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(diazadibenzoazulene pharmaceuticals for the treatment of central nervous system diseases)

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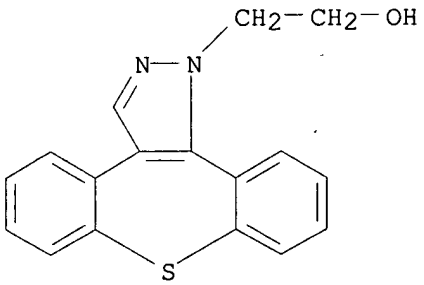

RN 629654-01-9 HCAPLUS
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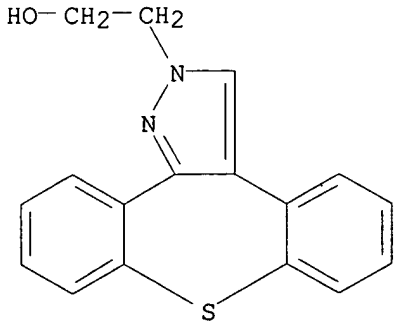

RN 629654-03-1 HCAPLUS
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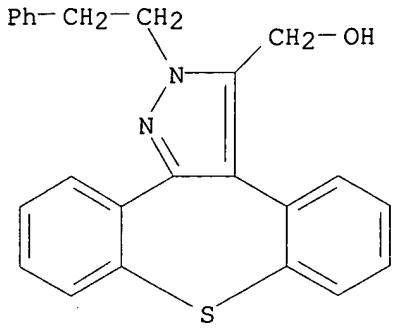

RN 629654-05-3 HCAPLUS
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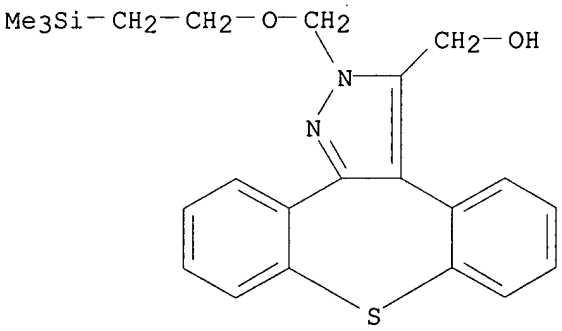

RN 629654-09-7 HCAPLUS
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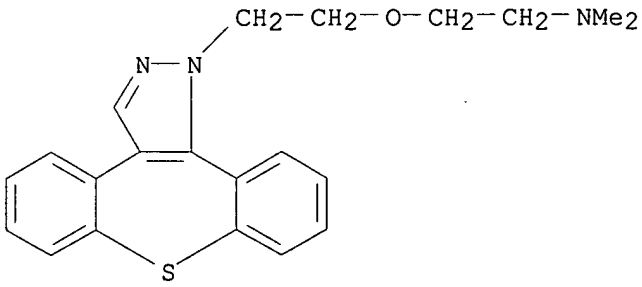

RN 629654-10-0 HCAPLUS
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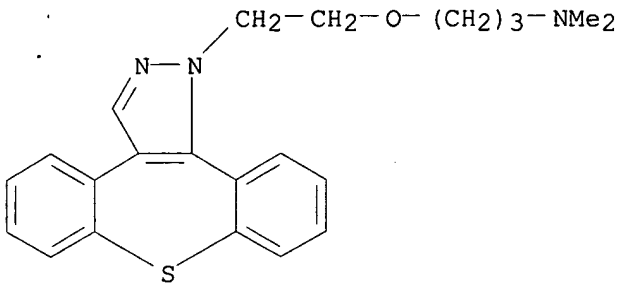
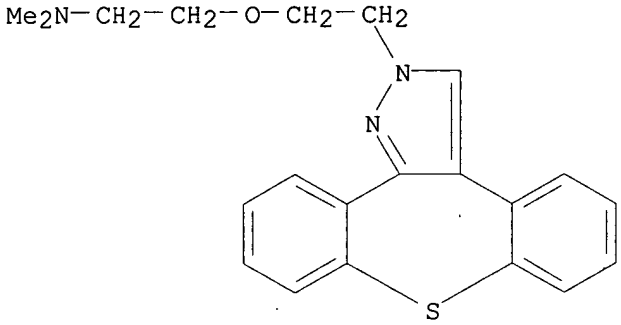


RN 629654-11-1 HCAPLUS
CN Ethanamine, 2-[2-(2H-dibenzo[2,3:6,7]thiepino[4,5-c]pyrazol-2-yl)ethoxy]-N,N-dimethyl- (CA INDEX NAME)



RN 629654-12-2 HCAPLUS
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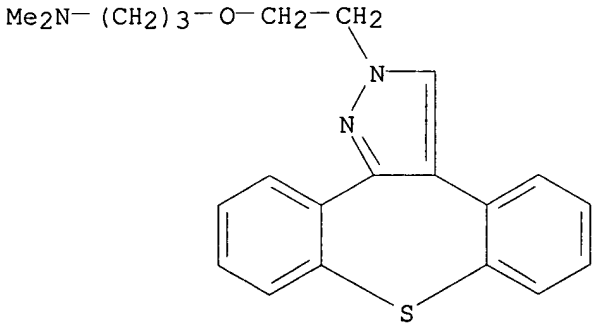

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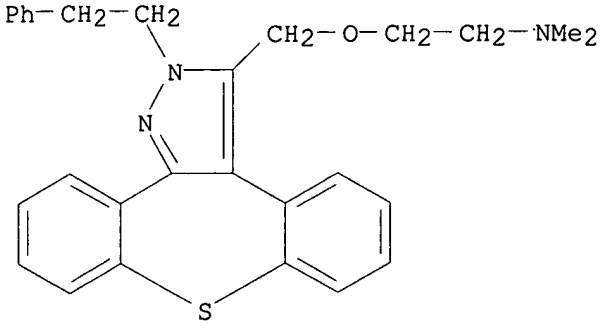

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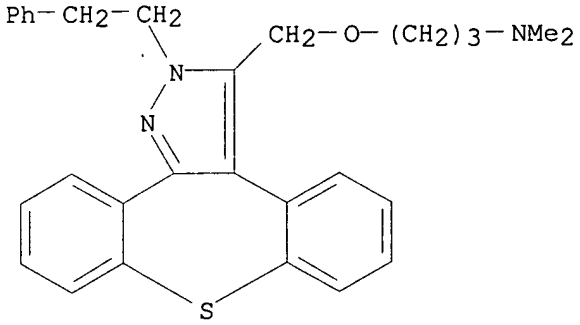

RN 629654-23-5 HCAPLUS
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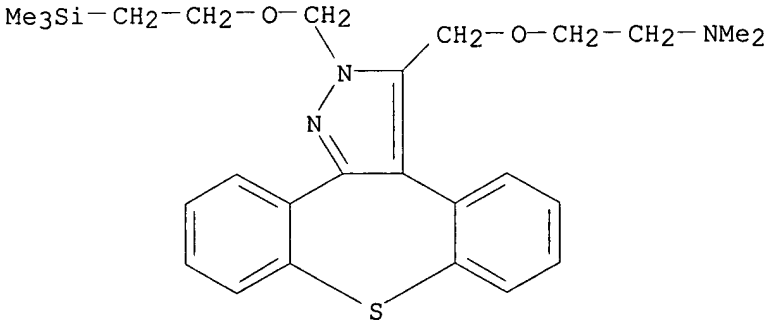

RN 629654-24-6 HCAPLUS
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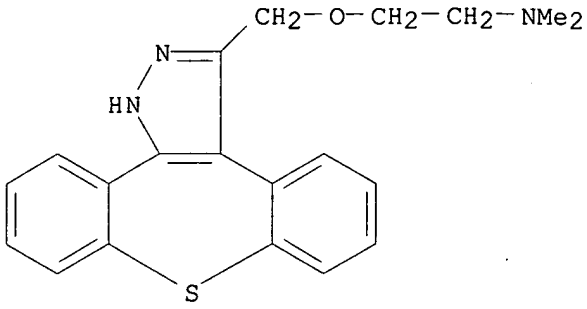

RN 629654-25-7 HCAPLUS
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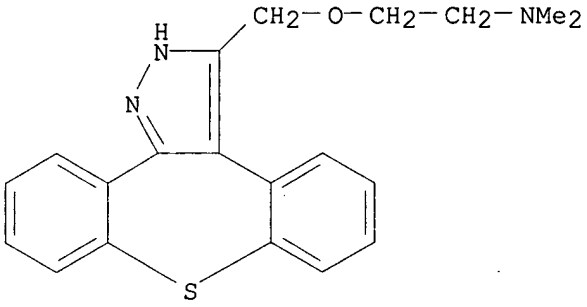

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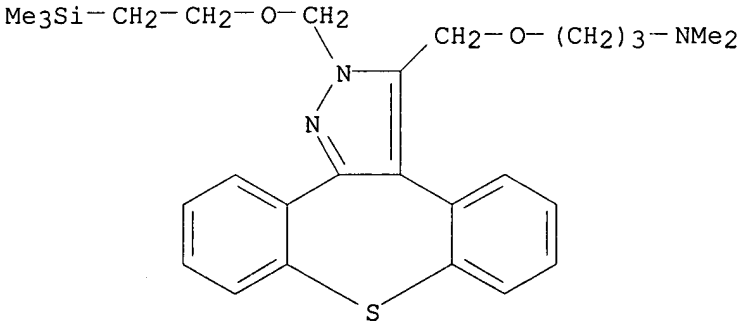

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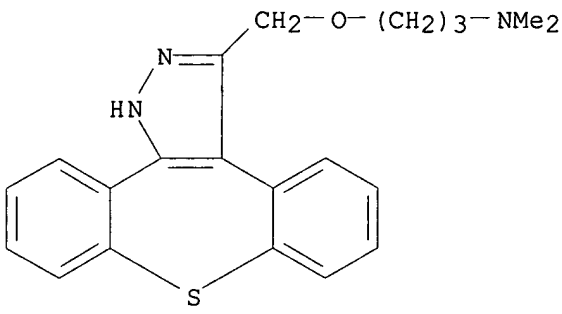

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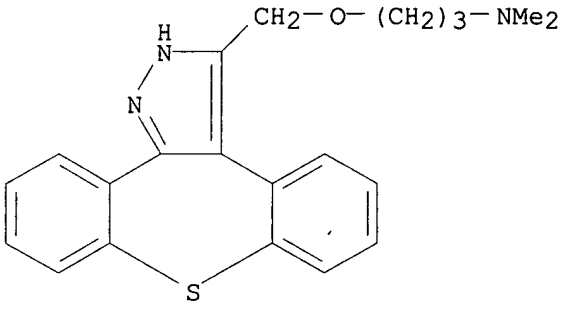
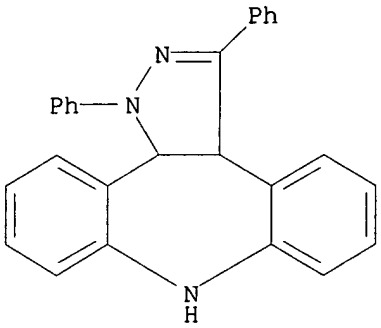


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2004:202758 HCAPLUS
DOCUMENT NUMBER: 142:176618
TITLE: Product subclass 6: benzazepines and their group 15 analogues
AUTHOR(S): Meigh, J.-P. K.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2004), 17, 825-927
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Methods for preparing benzazepines and their Group 15 analogs are reviewed including cyclization, ring transformation, aromatization and substituent modification.
IT **85008-85-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzazepine and their Group 15 analogs via cyclization, ring transformation, aromatization and substituent modification)
RN 85008-85-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl- (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)
REFERENCE COUNT: 234 THERE ARE 234 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2003:951029 HCAPLUS
DOCUMENT NUMBER: 140:16724
TITLE: Preparation of 1,2-Diazadibenzoazulenes as tumor necrosis factor inhibitors
INVENTOR(S): Mercep, Mladen; Mesic, Milan; Pesic, Dijana
PATENT ASSIGNEE(S): Pliva D.D., Croatia; Pliva Istrazivacki Inst. D.O.O.
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003099822	A2	20031204	WO 2003-HR22	20030520
WO 2003099822	A3	20050929		
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AU 2003232368	A1	20031212	AU 2003-232368	20030520
CN 1671712	A	20050921	CN 2003-816704	20030520
EP 1587807	A2	20051026	EP 2003-755234	20030520
EP 1587807	A3	20051116		
EP 1587807	B1	20080618		
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JP 2006500322	T	20060105	JP 2004-507479	20030520
AT 398621	T	20080715	AT 2003-755234	20030520
ES 2306888	T3	20081116	ES 2003-755234	20030520

IN 2004CN02879	A	20060217	IN 2004-CN2879		20041217
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PRIORITY APPLN. INFO.:			HR 2002-452	A	20020523
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OTHER SOURCE(S): MARPAT 140:16724

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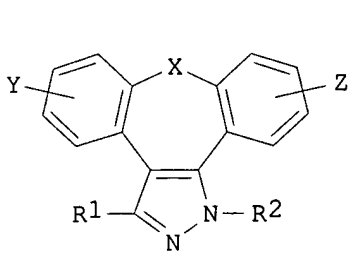

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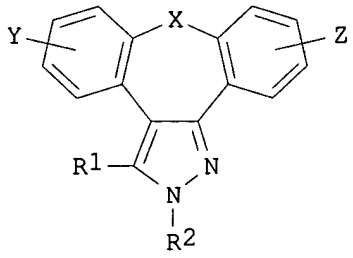

II

AB The present invention relates to 1,2-diazadibenzoazulene derivs. I and II [X = CH2, O, S, SO, SO2, NR; Y, Z = independently halo, C1-4 alkyl, C2-4 alkenyl, C2-4 alkynyl, halo-C1-4 alkyl, OH, C1-4 alkoxy, CF3CO, 1-4 alkanoyl, amino, amino-C1-4 alkyl, N-(C1-4 alkyl)amino, N,N-di(C1-4 alkyl)amino, SH, C1-4 alkylthio, SO2, C1-4 alkylsulfonyl, SO, C1-4 alkylsulfinyl, CO2H, C1-4 alkoxycarbonyl, CN, NO2; R = H, protecting group; R1 = halo, (un)substituted heteroaryl or heterocycle, OH, C1-7 alkoxy, aryloxy, amino, (CH2)mQ1(CH2)nQ2NR3R4, etc.; R2 = H, (un)substituted 1-7 alkyl, aryl, protecting group, CHO, 1-7 alkanoyl, C1-7 alkoxycarbonyl, aroyl, arylalkyl, etc; R3, R4 = H, C1-4 alkyl, aryl; NR3R4 = (un)substituted heterocycle, heteroaryl; n, m = 0-3; Q1, Q2 = O, S, CY1Y2, NY1, CY1:CH, C.tplbond.C; Y1, Y2 = H, halo, (un)substituted C1-4 alkyl, aryl, OH, C1-4 alkoxy, etc.] to their pharmacol. acceptable salts and solvates, to processes and intermediates for the preparation thereof as well as to their antiinflammatory actions, especially to the inhibition of tumor necrosis factor-x (TNF-(x)) production and the inhibition of interleukin-1 (IL-1) production as well as to their analgetic action. Thus, 2-(8-Oxa-1,2-diazadibenzo[e,h]azulen-1-yl)ethanol and 2-(8-Oxa-1,2-diazadibenzo[e,h]azulen-2-yl)ethanol were prepared and isolated by reacting 1,1-dimethylaminomethylene-1H-dibenzo[b,f]oxepin-10-one with ethanol hydrazine at a temperature 0-5°C in ethanol for 2 h.

IT **629653-82-3P 629653-85-6P 629653-88-9P**
629653-90-3P 629653-93-6P 629653-96-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(in preparation of 1,2-diaza-dibenzoazulene derivs. as inhibitors of tumor necrosis factor)

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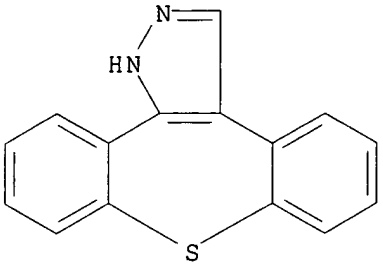

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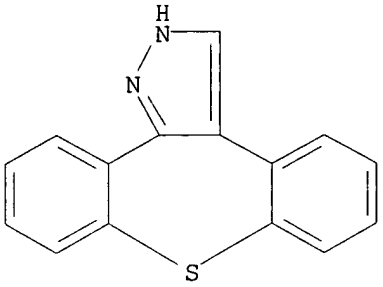

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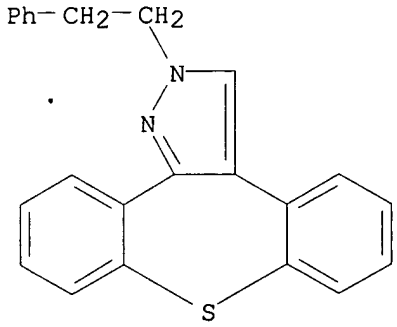

RN 629653-90-3 HCAPLUS
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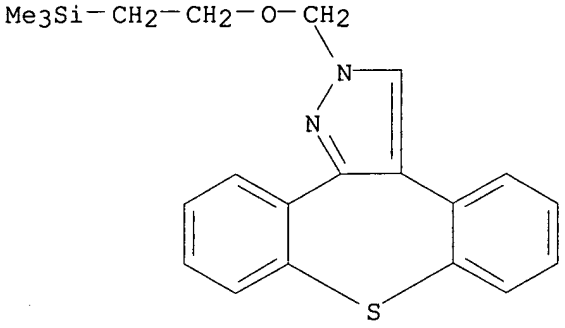

RN 629653-93-6 HCAPLUS
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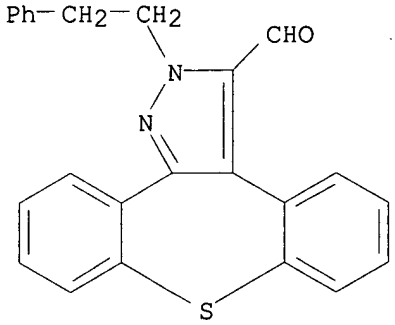

RN 629653-96-9 HCAPLUS
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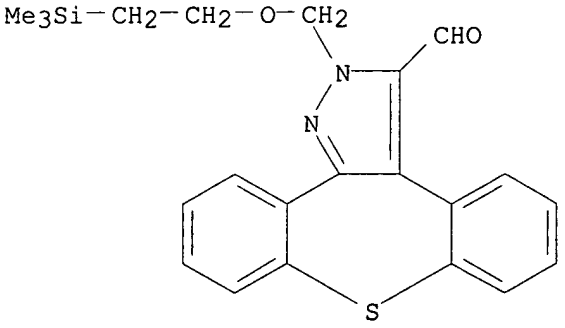

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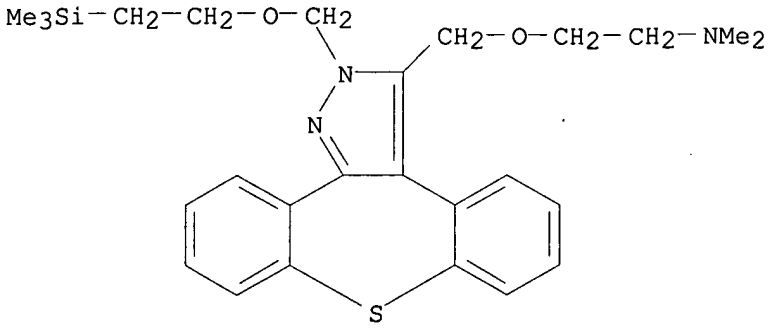
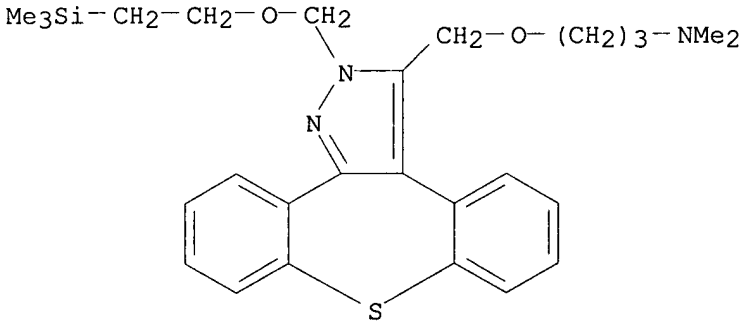
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1,2-diaza-dibenzoazulene derivs. as inhibitors of tumor necrosis factor)
RN 629654-23-5 HCAPLUS

CN Ethanamine, N,N-dimethyl-2-[[2-[[2-(trimethylsilyl)ethoxy]methyl]-2H-dibenzo[2,3:6,7]thiepino[4,5-c]pyrazol-3-yl]methoxy]- (CA INDEX NAME)



RN 629654-26-8 HCAPLUS
CN 1-Propanamine, N,N-dimethyl-3-[[2-[[2-(trimethylsilyl)ethoxy]methyl]-2H-dibenzo[2,3:6,7]thiepino[4,5-c]pyrazol-3-yl]methoxy]- (CA INDEX NAME)



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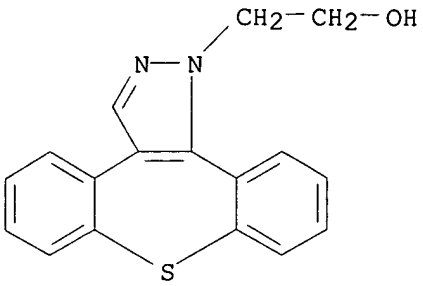
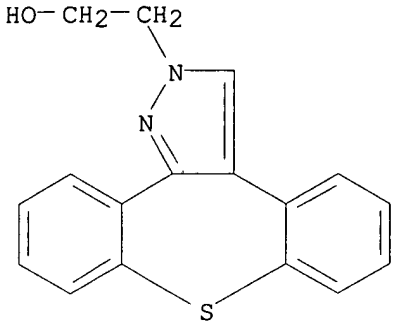
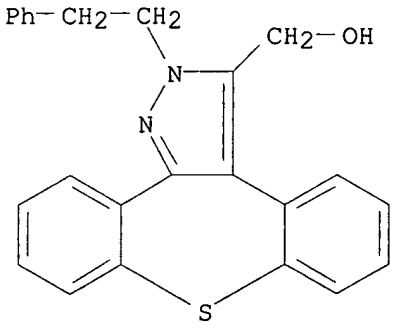
629654-05-3P **629654-09-7P** **629654-10-0P**
629654-11-1P **629654-12-2P** **629654-15-5P**
629654-16-6P **629654-24-6P** **629654-25-7P**
629654-27-9P **629654-28-0P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1,2-diaza-dibenzoazulene derivs. as inhibitors of tumor necrosis factor)
RN 629653-99-2 HCAPLUS
CN 1H-Dibenzo[2,3:6,7]thiepino[4,5-c]pyrazole-1-ethanol (CA INDEX NAME)



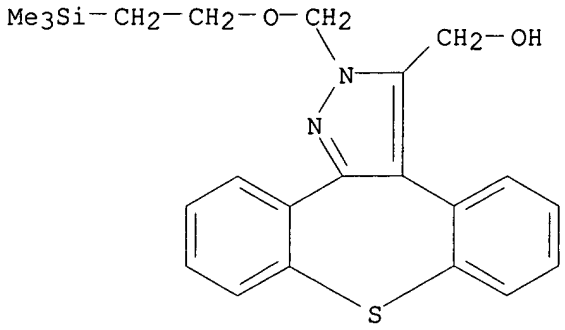
RN 629654-01-9 HCAPLUS
CN 2H-Dibenzo[2,3:6,7]thiepino[4,5-c]pyrazole-2-ethanol (CA INDEX NAME)



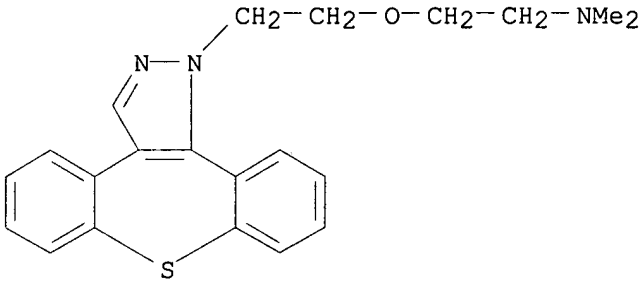
RN 629654-03-1 HCAPLUS
CN 2H-Dibenzo[2,3:6,7]thiepino[4,5-c]pyrazole-3-methanol, 2-(2-phenylethyl)-
(CA INDEX NAME)



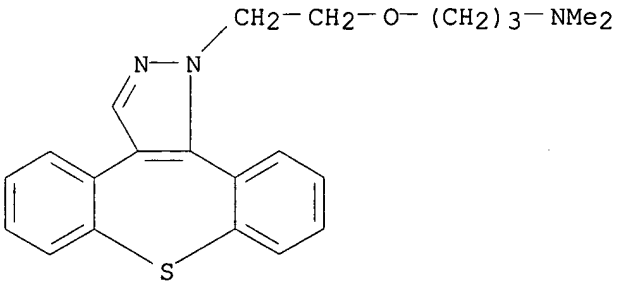
RN 629654-05-3 HCAPLUS
CN 2H-Dibenzo[2,3:6,7]thiepino[4,5-c]pyrazole-3-methanol,
2-[[2-(trimethylsilyl)ethoxy]methyl]- (CA INDEX NAME)



RN 629654-09-7 HCAPLUS
CN Ethanamine, 2-[2-(1H-dibenzo[2,3:6,7]thiepino[4,5-c]pyrazol-1-yl)ethoxy]-N,N-dimethyl- (CA INDEX NAME)



RN 629654-10-0 HCAPLUS
CN 1-Propanamine, 3-[2-(1H-dibenzo[2,3:6,7]thiepino[4,5-c]pyrazol-1-yl)ethoxy]-N,N-dimethyl- (CA INDEX NAME)



RN 629654-11-1 HCAPLUS
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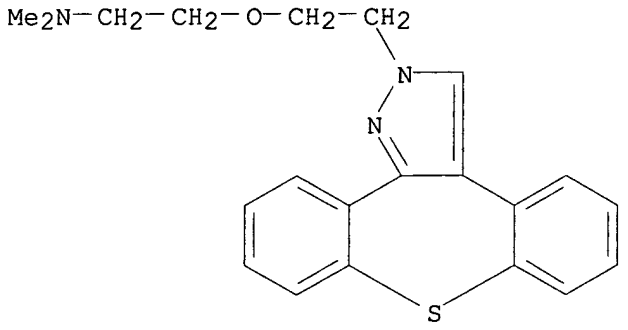

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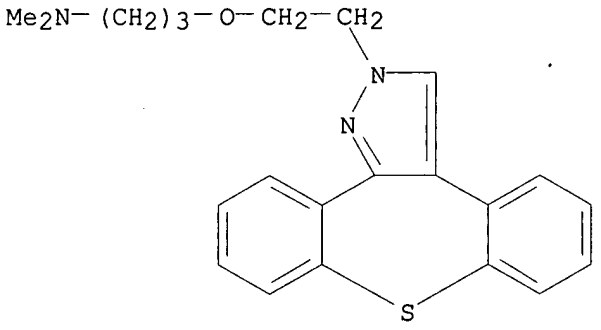

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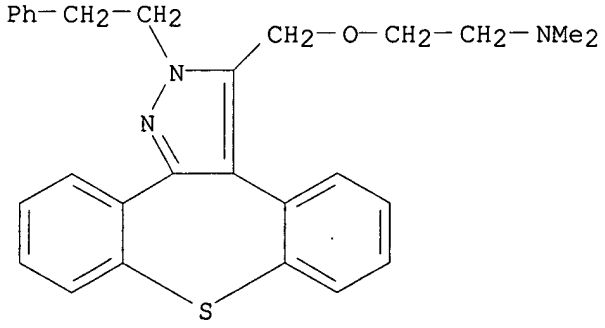

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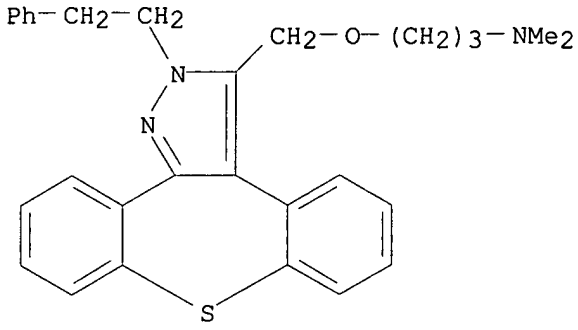

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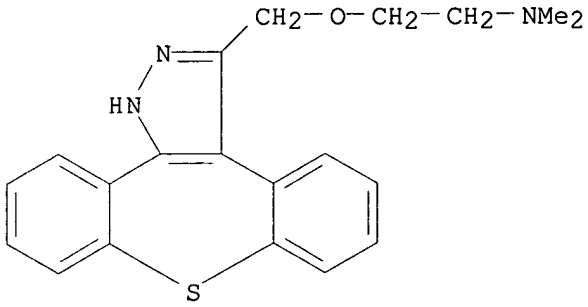

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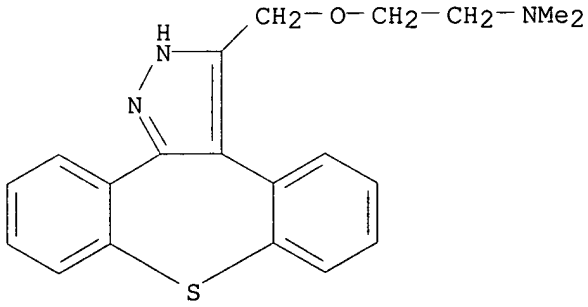

RN 629654-27-9 HCAPLUS
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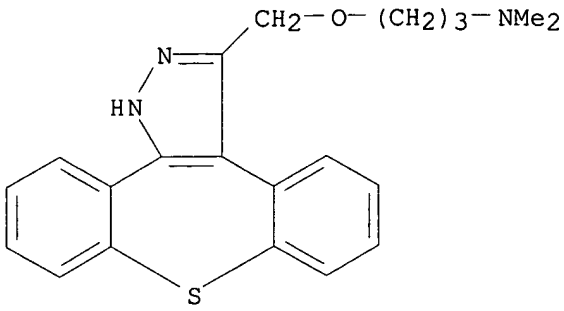

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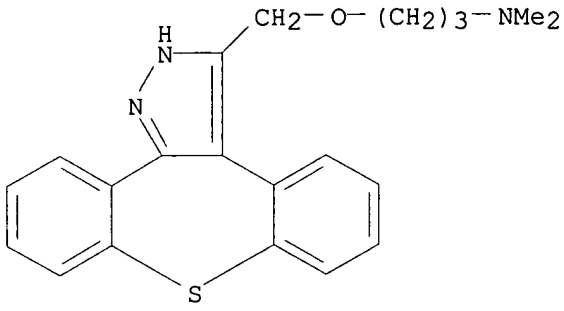

OS.CITING REF COUNT: 5 THERE ARE 5 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2002:928245 HCAPLUS
DOCUMENT NUMBER: 138:14055
TITLE: Preparation of substituted thioacetamides for treatment of sleep disorders
INVENTOR(S): Bacon, Edward R.; Chatterjee, Sankar; Dunn, Derek; Mallamo, John P.; Miller, Matthew S.; Tripathy, Rabindranath; Vaught, Jeffry L.
PATENT ASSIGNEE(S): Cephalon, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 52 pp., Cont.-in-part of U.S. Ser. No. 855,228.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020183334	A1	20021205	US 2001-14645	20011026
US 6670358	B2	20031230		
US 20020045629	A1	20020418	US 2001-855228	20010515
US 6492396	B2	20021210		

CA 2462206	A1	20030508	CA 2002-2462206		20021025
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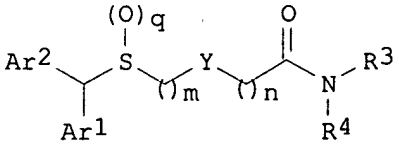

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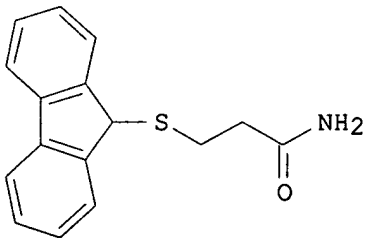


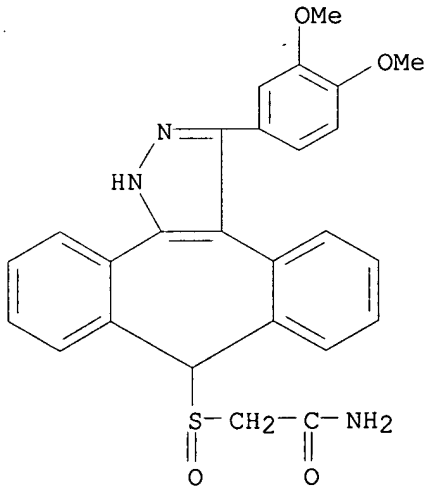
II

AB Title compds. I [Ar1-2 = (hetero)aryl; Y = alkylene, alkyl, (hetero)arylene, cycloalkylene, O, SO0-2, etc.; R3-4 = H, alkyl, OH, etc.; m, n = 0-3; q = 0-2] were prepared For instance, thiourea and 9-hydroxyfluorene were reacted (HBraq, 100-105°, 30 min) to afford the corresponding thiouronium salt. This was treated with NaOHaq and 3-bromopropionic acid to afford the sulfide-carboxylic acid and subsequently treated with SOCl2/NH4OH to give II. Selected example compds. possessed wake-promoting activity (rats). I are useful in the treatment of sleep disorders, Parkinson's disease, etc.

IT **477727-99-4P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted thioacetamides for treatment of sleep disorders)

RN 477727-99-4 HCAPLUS

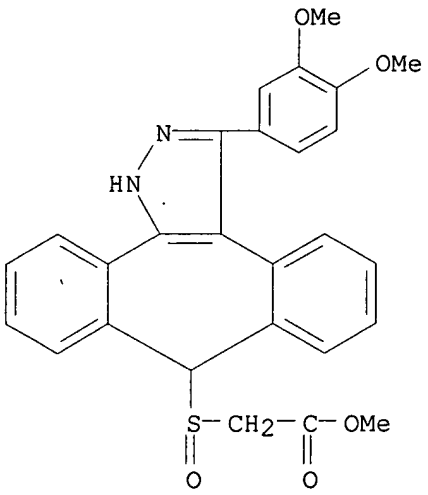
CN Acetamide, 2-[[3-(3,4-dimethoxyphenyl)-1,8-dihydrodibenzo[3,4:6,7]cyclohepta[1,2]pyrazol-8-yl]sulfinyl]- (CA INDEX NAME)



IT **477728-19-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted thioacetamides for treatment of sleep disorders)

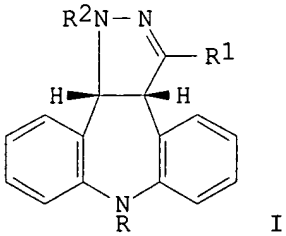
RN 477728-19-1 HCAPLUS

CN Acetic acid, 2-[[3-(3,4-dimethoxyphenyl)-1,8-dihydrodibenzo[3,4:6,7]cyclohepta[1,2]pyrazol-8-yl]sulfinyl]-, methyl ester (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (5 CITINGS)

L3 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1988:630883 HCAPLUS
DOCUMENT NUMBER: 109:230883
ORIGINAL REFERENCE NO.: 109:38185a,38188a
TITLE: Synthesis of 1,3a,8,12b-tetrahydrodibenzo[b,f]pyrazolo[3,4-d]azepine derivatives
AUTHOR(S): Schulz, Hans Joachim; Jugelt, Werner; Grubert, Lutz
CORPORATE SOURCE: Sekt. Chem., Humboldt-Univ., Berlin, DDR-1040, Ger. Dem. Rep.
SOURCE: Zeitschrift fuer Chemie (1988), 28(5), 181-2
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 109:230883
GI



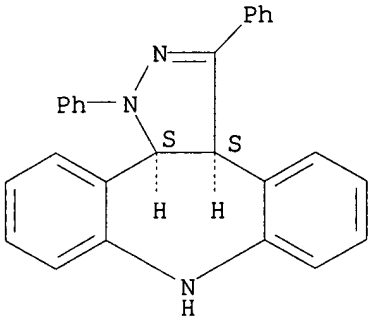
I

AB The title compds. I [R = H, Me, Ac, CONH2, COCl; R1 = Ph, Ac, CO2Me, Me, 4-ClC6H4, 4-MeOC6H4; R2 = Ph, 4-MeC6H4, 2,4-(O2N)2C6H3] were obtained by reaction of the dibenzazepines with R1CCl:NNHR2.

IT **117600-87-0P** **117600-88-1P** **117600-89-2P**
117600-90-5P **117600-91-6P** **117600-92-7P**
117600-93-8P **117600-94-9P** **117600-95-0P**
117600-96-1P **117600-97-2P** **117600-98-3P**
117600-99-4P **117601-00-0P** **117601-01-1P**

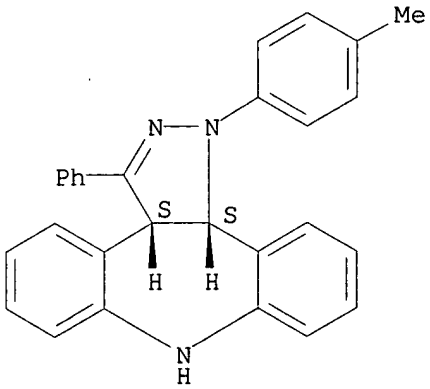
117601-02-2P 117601-03-3P 117601-04-4P
117601-05-5P 117601-06-6P 117601-07-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 117600-87-0 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



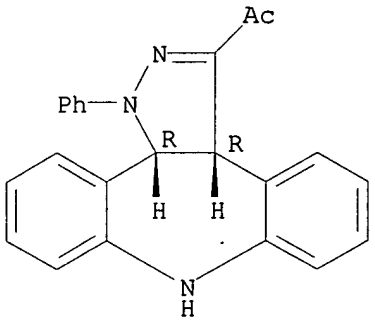
RN 117600-88-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1-(4-methylphenyl)-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



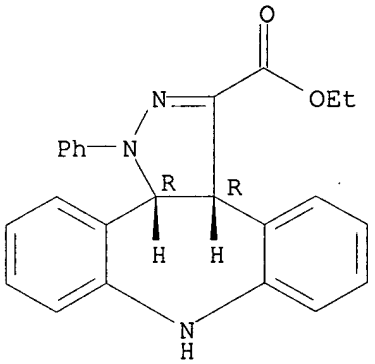
RN 117600-89-2 HCAPLUS
CN Ethanone, 1-(1,3a,8,12b-tetrahydro-1-phenyldibenzo[b,f]pyrazolo[3,4-d]azepin-3-yl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



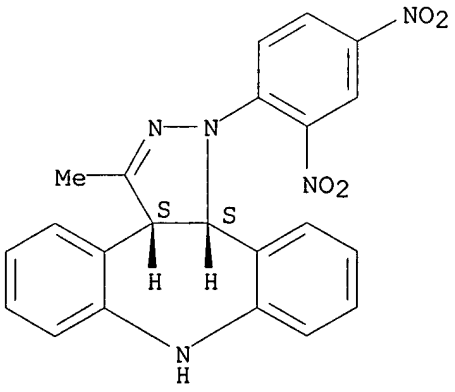
RN 117600-90-5 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-3-carboxylic acid, 1,3a,8,12b-tetrahydro-1-phenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 117600-91-6 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1-(2,4-dinitrophenyl)-1,3a,8,12b-tetrahydro-3-methyl-, cis- (9CI) (CA INDEX NAME)

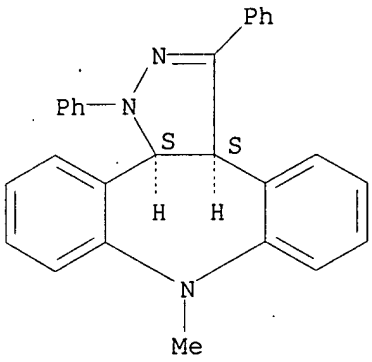
Relative stereochemistry.



RN 117600-92-7 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine,

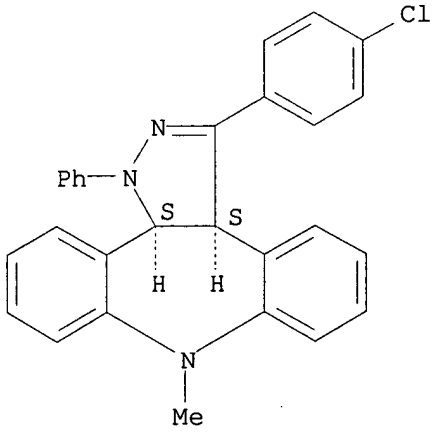
1,3a,8,12b-tetrahydro-8-methyl-1,3-diphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



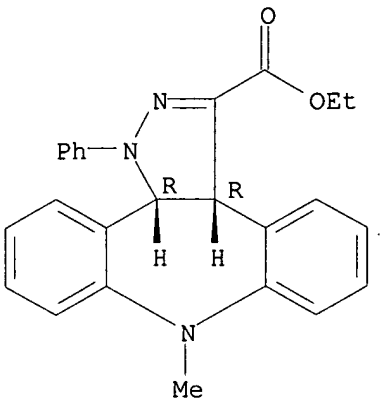
RN 117600-93-8 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine,
3-(4-chlorophenyl)-1,3a,8,12b-tetrahydro-8-methyl-1-phenyl-, cis- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



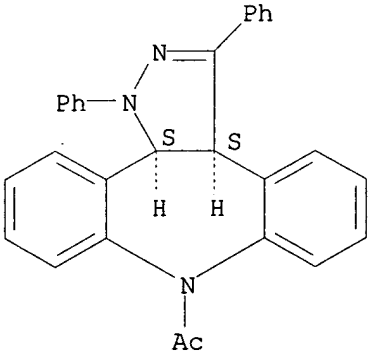
RN 117600-94-9 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-3-carboxylic acid,
1,3a,8,12b-tetrahydro-8-methyl-1-phenyl-, ethyl ester, cis- (9CI) (CA
INDEX NAME)

Relative stereochemistry.



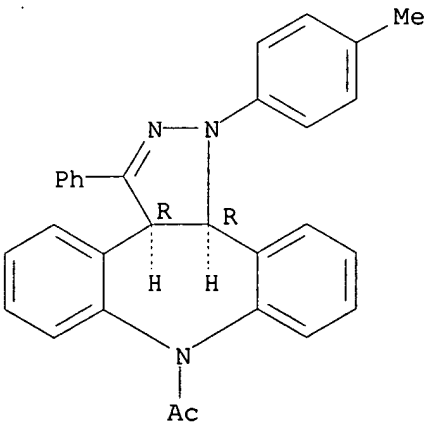
RN 117600-95-0 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine,
8-acetyl-1,3a,8,12b-tetrahydro-1,3-diphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



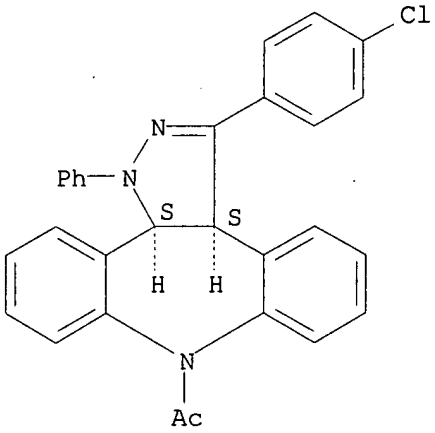
RN 117600-96-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine,
8-acetyl-1,3a,8,12b-tetrahydro-1-(4-methylphenyl)-3-phenyl-, cis- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



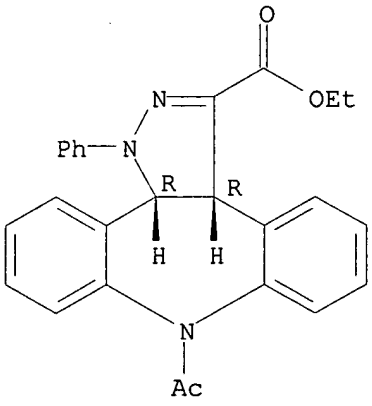
RN 117600-97-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 8-acetyl-3-(4-chlorophenyl)-1,3a,8,12b-tetrahydro-1-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



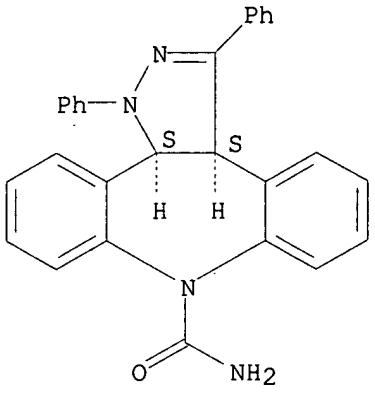
RN 117600-98-3 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-3-carboxylic acid, 8-acetyl-1,3a,8,12b-tetrahydro-1-phenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



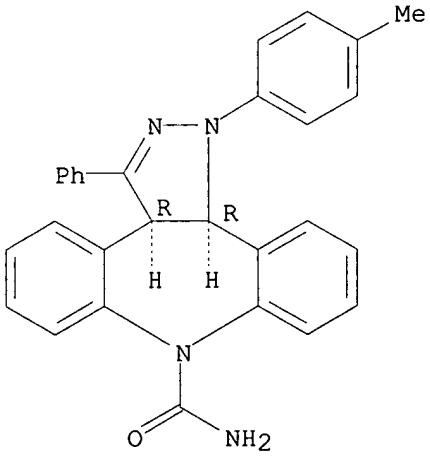
RN 117600-99-4 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carboxamide, 3a,12b-dihydro-1,3-diphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



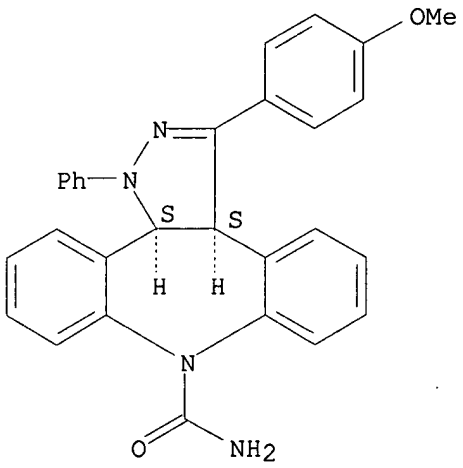
RN 117601-00-0 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carboxamide, 3a,12b-dihydro-1-(4-methylphenyl)-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



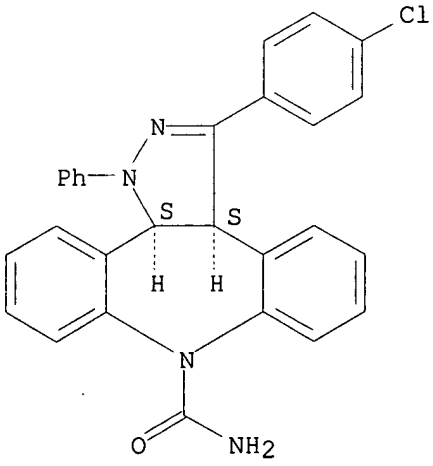
RN 117601-01-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carboxamide, 3a,12b-dihydro-3-(4-methoxyphenyl)-1-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



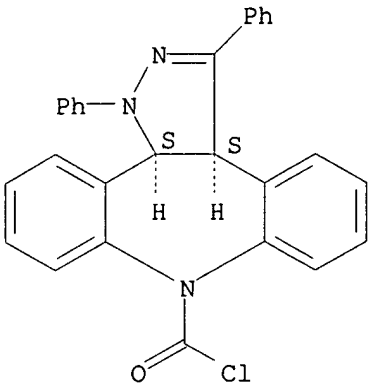
RN 117601-02-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carboxamide, 3-(4-chlorophenyl)-3a,12b-dihydro-1-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



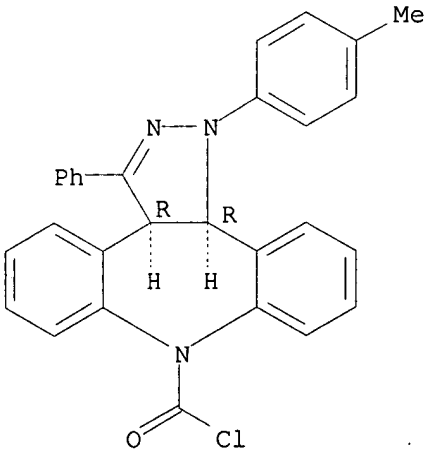
RN 117601-03-3 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carbonyl chloride, 3a,12b-dihydro-1,3-diphenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



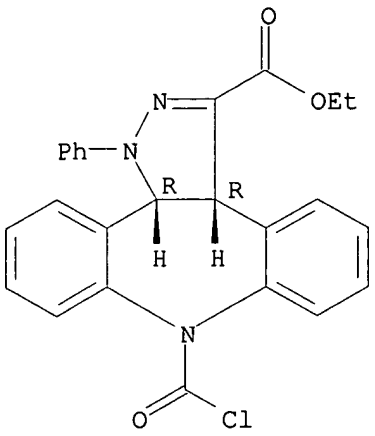
RN 117601-04-4 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carbonyl chloride, 3a,12b-dihydro-1-(4-methylphenyl)-3-phenyl-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



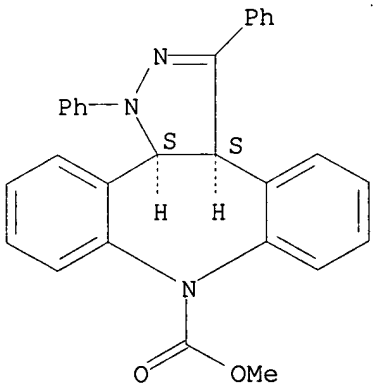
RN 117601-05-5 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-3-carboxylic acid, 8-(chlorocarbonyl)-1,3a,8,12b-tetrahydro-1-phenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



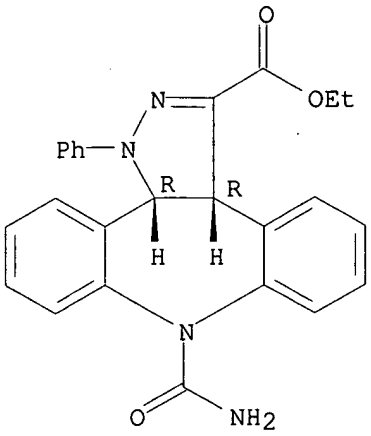
RN 117601-06-6 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-8(1H)-carboxylic acid, 3a,12b-dihydro-1,3-diphenyl-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



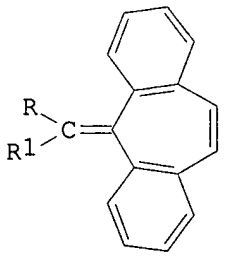
RN 117601-07-7 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine-3-carboxylic acid, 8-(aminocarbonyl)-1,3a,8,12b-tetrahydro-1-phenyl-, ethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

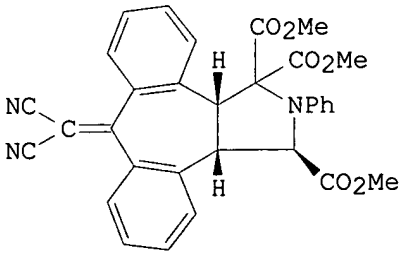


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L3 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1985:405738 HCAPLUS
DOCUMENT NUMBER: 103:5738
ORIGINAL REFERENCE NO.: 103:1035a,1038a
TITLE: Regioselectivity of 1,3-dipolar cycloaddition. Reactions of 2,3:6,7-dibenzoheptafulvenes with some dipoles
AUTHOR(S): Fichou, D.; Tonnard, F.; Toupet, L.; Carrie, R.
CORPORATE SOURCE: Dep. Phys. Crist. Chim. Struct., CNRS, Rennes, 35042, Fr.
SOURCE: Tetrahedron (1984), 40(24), 5121-33
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



I



II

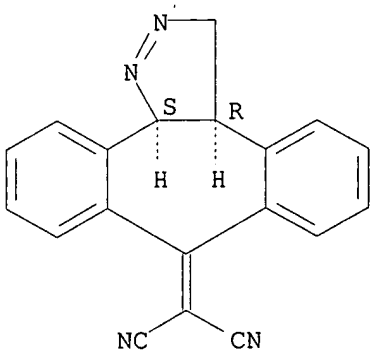
AB The addition of 1,3-dipoles (e.g., diazoalkanes, p-ClC6H4C.tplbond.NO, and azomethine ylides) to 2,3:6,7-dibenzo-heptafulvenes I (R = R1 = CN; R = CN, R1 = H, CO2Me; R = CO2Me, R1 = H) occurs exclusively at the endocyclic double bond, leading resp. to pyrazolines, isoxazolines and pyrrolidines. This regiospecificity is due to steric factors which are discussed using Sustmann's (1972) variation perturbation theory. The crystallog. of the pyrrolidine II is also discussed.

IT **96606-41-6P** **96606-42-7P** **96606-43-8P**
96606-44-9P **96606-45-0P** **96606-46-1P**
96606-47-2P **96606-48-3P** **96606-52-9P**

96623-05-1P 96623-06-2P 96647-47-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

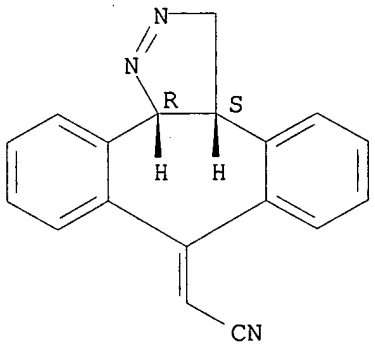
RN 96606-41-6 HCAPLUS
CN Propanedinitrile, (3a,12b-dihydrodibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



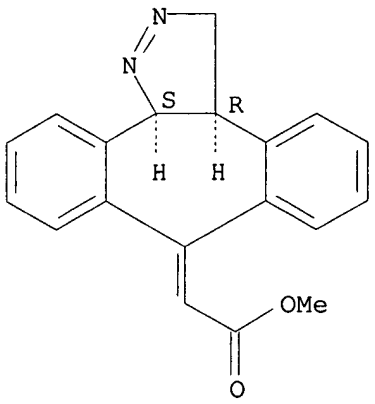
RN 96606-42-7 HCAPLUS
CN Acetonitrile, (3a,12b-dihydrodibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



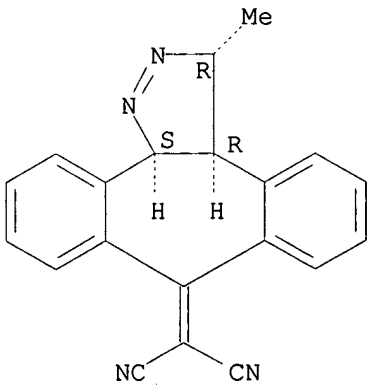
RN 96606-43-8 HCAPLUS
CN Acetic acid, (3a,12b-dihydrodibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



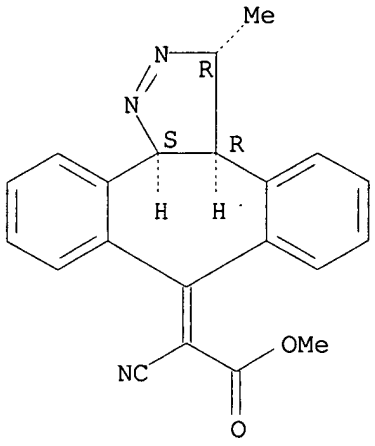
RN 96606-44-9 HCAPLUS
CN Propanedinitrile, (3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, (3α,3aα,12bα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

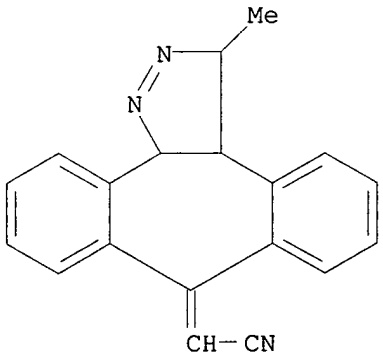


RN 96606-45-0 HCAPLUS
CN Acetic acid, cyano(3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, methyl ester, (3α,3aα,12bα)- (9CI) (CA INDEX NAME)

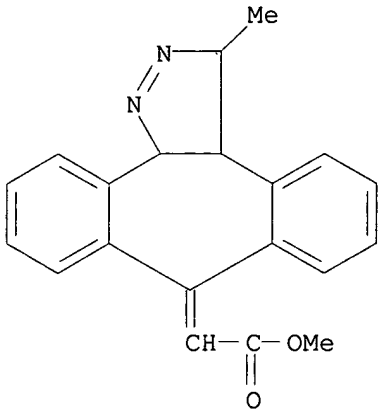
Relative stereochemistry.
Double bond geometry unknown.



RN 96606-46-1 HCAPLUS
CN Acetonitrile, (3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, (3α,3aα,12bα)- (9CI) (CA INDEX NAME)

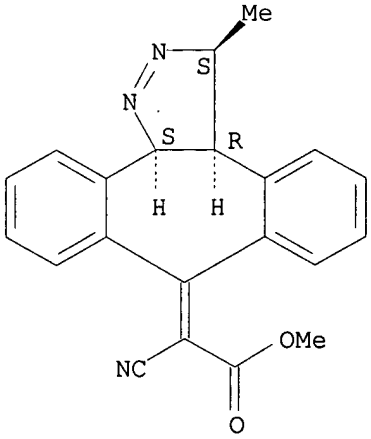


RN 96606-47-2 HCAPLUS
CN Acetic acid, (3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, methyl ester, (3α,3aα,12bα)- (9CI) (CA INDEX NAME)

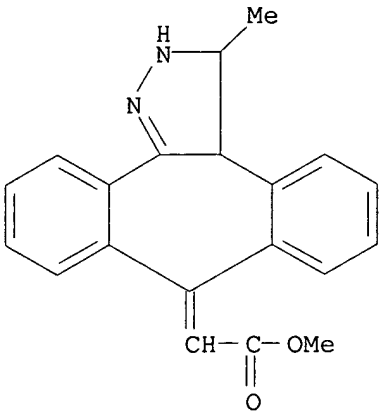


RN 96606-48-3 HCAPLUS
CN Acetic acid, cyano(3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, methyl ester, (3α,3aβ,12bβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

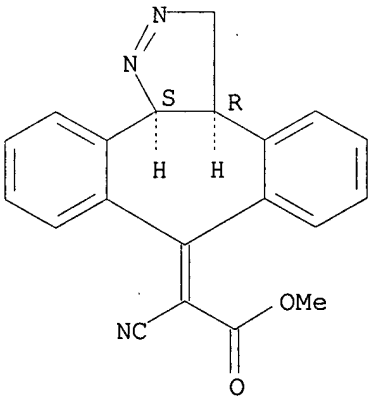


RN 96606-52-9 HCAPLUS
CN Acetic acid, 2-(3,3a-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2]pyrazol-8(2H)-ylidene)-, methyl ester (CA INDEX NAME)

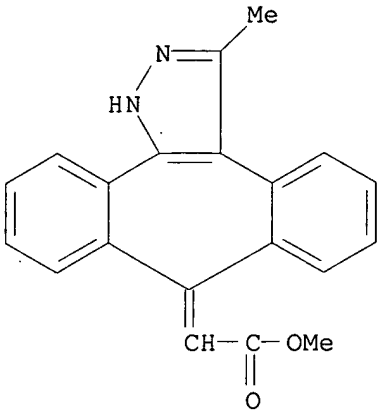


RN 96623-05-1 HCAPLUS
CN Acetic acid, cyano(3a,12b-dihydrodibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, methyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

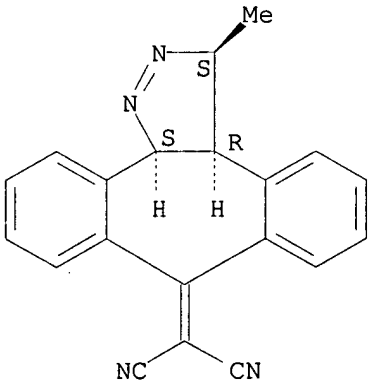


RN 96623-06-2 HCAPLUS
CN Acetic acid, 2-(3-methyldibenzo[3,4:6,7]cyclohepta[1,2]pyrazol-8(1H)-ylidene)-, methyl ester (CA INDEX NAME)



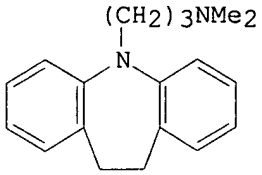
RN 96647-47-1 HCAPLUS
CN Propanedinitrile, (3a,12b-dihydro-3-methyldibenzo[3,4:6,7]cyclohepta[1,2-c]pyrazol-8(3H)-ylidene)-, (3α,3aβ,12bβ)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L3 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1984:403202 HCAPLUS
DOCUMENT NUMBER: 101:3202
ORIGINAL REFERENCE NO.: 101:559a,562a
TITLE: Determination of the radioprotective activity of imipramine analogs
AUTHOR(S): Gansser, C.; Marcot, B.; Viel, C.; Fatome, M.; Laval, J. D.
CORPORATE SOURCE: Lab. Pharm. Chim., Fac. Pharm., Chatenay-Malabry, F 92290, Fr.
SOURCE: Annales Pharmaceutiques Francaises (1983), 41(5), 465-71
CODEN: APFRAD; ISSN: 0003-4509
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



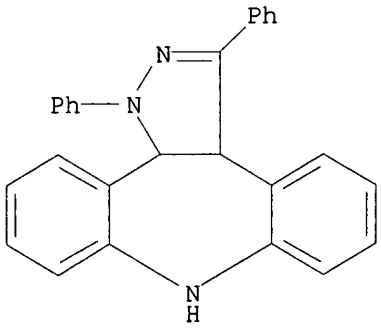
I

AB The radioprotective activity of analogs of imipramine (I) were examined The radioprotectant activity was studied in male albino mice exposed to γ-irradiation (0.3 Gy/min) and injected with 50-375 mg/kg i.p., and the results compared with AET. The I analogs containing pyridoazepine or azepinone had radioprotectant activity based on LD50/30, but were all inferior to AET.

IT **90358-73-9 90358-74-0 90358-75-1 90358-76-2**
RL: BIOL (Biological study)
(radioprotection by)

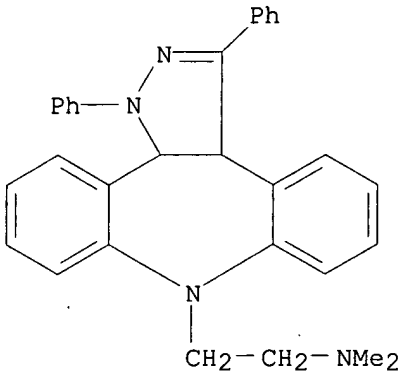
RN 90358-73-9 HCAPLUS

CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl-, hydrochloride (1:?) (CA INDEX NAME)



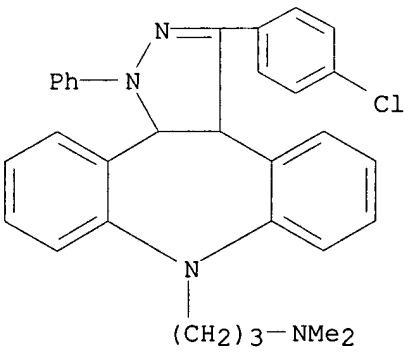
RN 90358-74-0 HCAPLUS

CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-ethanamine, 3a,12b-dihydro-N,N-dimethyl-1,3-diphenyl-, hydrochloride (1:?) (CA INDEX NAME)



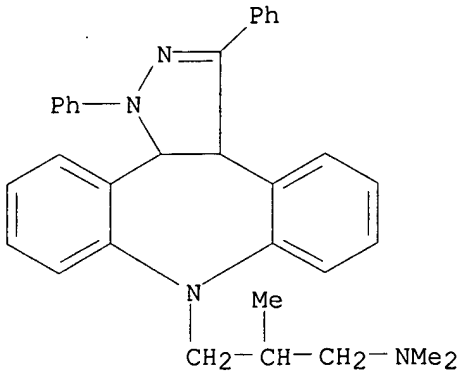
● x HCl

RN 90358-75-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, 3-(4-chlorophenyl)-3a,12b-dihydro-N,N-dimethyl-1-phenyl-, hydrochloride (1:?) (CA INDEX NAME)



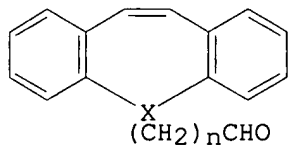
● x HCl

RN 90358-76-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, 3a,12b-dihydro-N,N,β-trimethyl-1,3-diphenyl-, hydrochloride (1:?) (CA INDEX NAME)

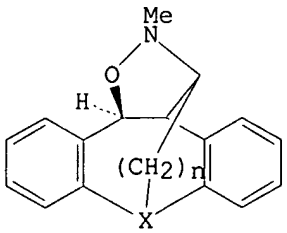


●x HCl

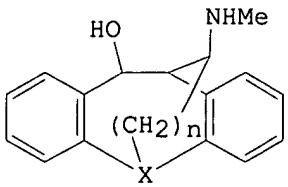
L3 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:505107 HCAPLUS
DOCUMENT NUMBER: 99:105107
ORIGINAL REFERENCE NO.: 99:16177a,16180a
TITLE: Intramolecular [3 + 2] cycloaddition routes to carbon-bridged dibenzocycloheptanes and dibenzazepines
AUTHOR(S): Confalone, Pat N.; Huie, Edward M.
CORPORATE SOURCE: Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE, 19898, USA
SOURCE: Journal of Organic Chemistry (1983), 48(18), 2994-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:105107
GI



I



II

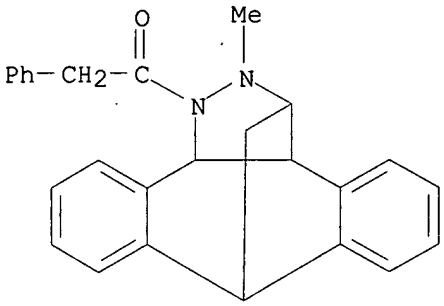


III

AB Treating aldehydes I (X = CH, N, n = 1; X = CH, n = 0) with MeNHOH gave bridged polycyclic isoxazolidones II, which on dissolving-metal reduction gave title compds. III. The reactions of I (X = CH, n = 1) with MeNHCH2CO2Et

and sarcosine Et ester are also described.

IT **86569-13-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 86569-13-3 HCAPLUS
CN Ethanone, 2-phenyl-1-(3,3a,8,12b-tetrahydro-2-methyl-3,8-methanodibenzo[3,4:6,7]cyclohepta[1,2]pyrazol-1(2H)-yl)- (CA INDEX NAME)

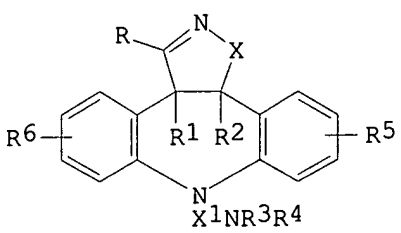


OS.CITING REF COUNT: 11 THERE ARE 11 CAPLUS RECORDS THAT CITE THIS RECORD (11 CITINGS)

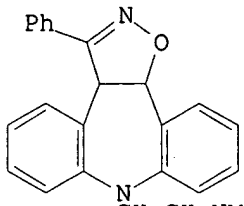
L3 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1983:143412 HCAPLUS
DOCUMENT NUMBER: 98:143412
ORIGINAL REFERENCE NO.: 98:21853a,21856a
TITLE: Dibenzazepine tetracyclic derivatives and pharmaceutical compositions containing them
INVENTOR(S): Viel, Claude; Marcot, Bernoud; Redeuilh, Gerard; Djiane, Alain; Cherqui, Jean
PATENT ASSIGNEE(S): Centre National de la Recherche Scientifique, Fr.
SOURCE: Eur. Pat. Appl., 54 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 63525	A1	19821027	EP 1982-400680		19820415
R: BE, CH, DE, FR, GB, IT, NL, SE					
FR 2504140	A1	19821022	FR 1981-7707		19810416
FR 2504140	B1	19831202			
JP 58088384	A	19830526	JP 1982-63793		19820416
PRIORITY APPLN. INFO.:			FR 1981-7707	A	19810416

OTHER SOURCE(S): CASREACT 98:143412; MARPAT 98:143412
GI



I



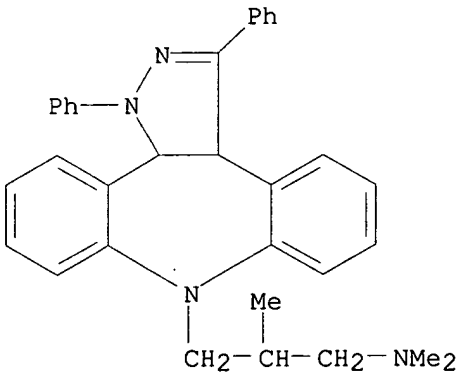
II

AB Azolodibenzazepines I (X = O, NR7; X1 = alkene; R = alkyl, Ph, substituted Ph; R1, R2 = H; R1R2 = bond, R3, R4 = H, alkyl, aralkyl; NR3R4 = heterocyclic; R5, R6 = H, alkyl, alkoxy, CF3, alkylenedioxy, OH, SH, OCCl3, OCF3, SCF3, amino, aminosulfonyl, cyano, NO2, CO2H, alkoxycarbonyl, carbamoyl, acyl, sulfinyl, sulfonyl; R7 = Ph, substituted Ph) were prepared Thus, dibenzazepine was treated with ClCH2CH2NMe2 and cyclized with PhCCl:NOH to give II. At 5 mg/kg i.p. II was antireserpine activity in mice. II gave 70% protection against phenylbenzoquine writhing in mice at 20 mg/kg i.p. It had an anticholinergic ED50 of 5 + 10-4 mg/mL in the isolated guinea pig ileum.

IT **85008-83-9P 85008-84-0P 85008-86-2P**
85008-87-3P 85008-90-8P 85008-94-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antidepressant activity of)

RN 85008-83-9 HCAPLUS

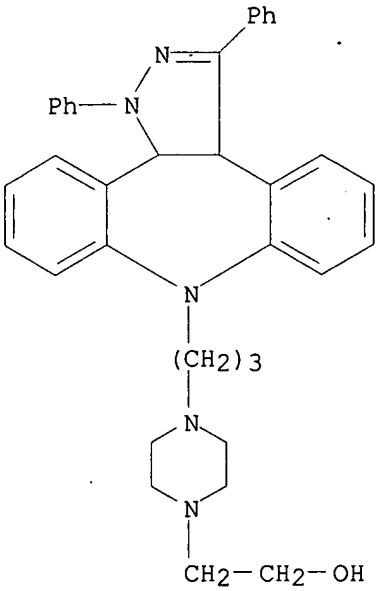
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, 3a,12b-dihydro-N,N,β-trimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



● HCl

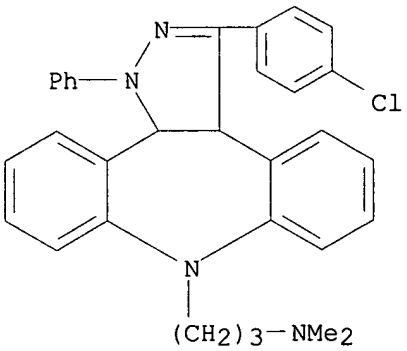
RN 85008-84-0 HCAPLUS

CN 1-Piperazineethanol, 4-[3-(3a,12b-dihydro-1,3-diphenyldibenzo[b,f]pyrazolo[4,3-d]azepin-8(1H)-yl)propyl]-, hydrochloride (1:1) (CA INDEX NAME)



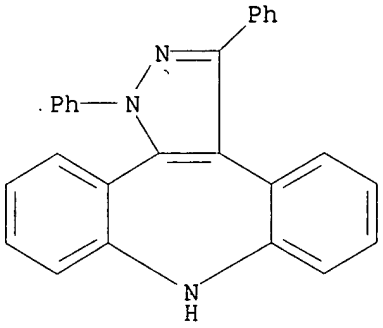
● HCl

RN 85008-86-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, 3-(4-chlorophenyl)-3a,12b-dihydro-N,N-dimethyl-1-phenyl-, hydrochloride (1:1) (CA INDEX NAME)

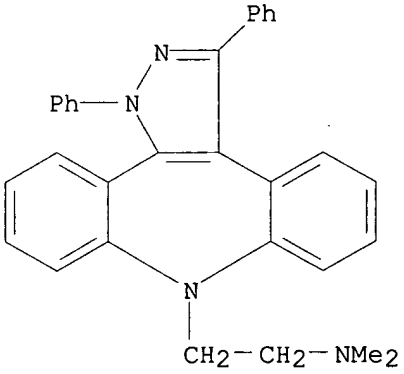


● HCl

RN 85008-87-3 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,8-dihydro-1,3-diphenyl- (CA INDEX NAME)

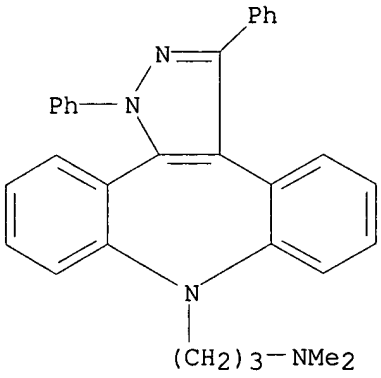


RN 85008-90-8 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-ethanamine, N,N-dimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



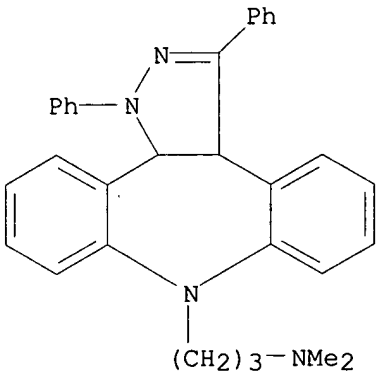
● HCl

RN 85008-94-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, N,N-dimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



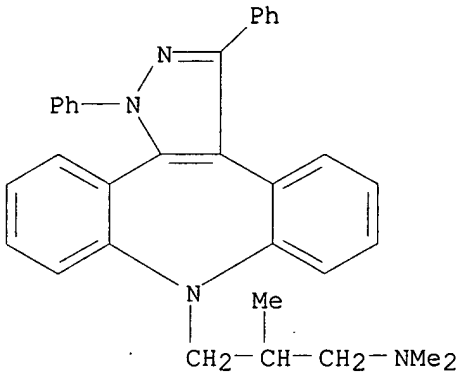
● HCl

IT **85008-81-7P 85008-91-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 85008-81-7 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, 3a,12b-dihydro-N,N-dimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



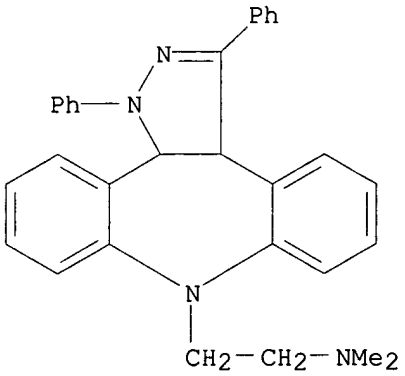
● HCl

RN 85008-91-9 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-propanamine, N,N,β-trimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



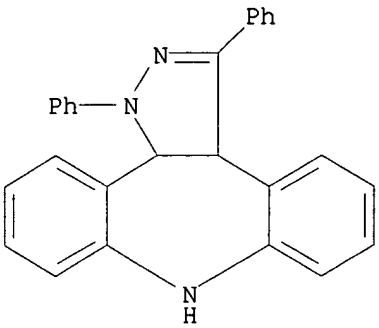
● HCl

IT **85008-82-8P 85008-85-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, dehydrogenation, and antidepressant activity of)
RN 85008-82-8 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine-8(1H)-ethanamine, 3a,12b-dihydro-N,N-dimethyl-1,3-diphenyl-, hydrochloride (1:1) (CA INDEX NAME)



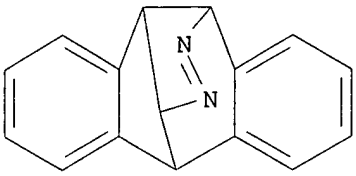
● HCl

RN 85008-85-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl- (CA INDEX NAME)

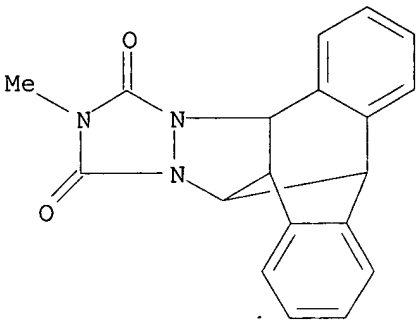


OS.CITING REF COUNT: 7 THERE ARE 7 CAPLUS RECORDS THAT CITE THIS RECORD (7 CITINGS)

L3 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1982:581459 HCAPLUS
DOCUMENT NUMBER: 97:181459
ORIGINAL REFERENCE NO.: 97:30345a,30348a
TITLE: Photochemical and thermal denitrogenations of azoalkanes as mechanistic probes for the diradical intermediates involved in the di-π-methane rearrangement of dibenzobarrelene
AUTHOR(S): Adam, Waldemar; De Lucchi, Ottorino; Peters, Karl; Peters, Eva Maria; Von Schnering, Hans Georg
CORPORATE SOURCE: Inst. Org. Chem., Univ. Wuerzburg, Wuerzburg, 8700, Fed. Rep. Ger.
SOURCE: Journal of the American Chemical Society (1982), 104(21), 5747-53
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:181459
GI For diagram(s), see printed CA Issue.
AB I and II were prepared from III and IV, resp., which, in turn, were obtained by reaction of dibenzobarrelene (V) with N-methyl-1,2,4-triazoline-3,5-dione. Thermolysis, direct photolysis at 350 and 254 nm, and Ph2CO sensitization leads to the diradicals VI (from I) and VII (from II), which are postulated intermediates in the di-π-methane rearrangement of V. The singlet-state diradicals lead to V and VIII as minor products and IX as the major product. Thus, the extent of retro-di-π-methane rearrangement of VII is small. Formation of X via rearrangement of VII to XI, a hitherto unrecognized di-π-methane route of V, takes place only to a very small extent in the 254-nm photolysis of II. Triplet-state VI and VIII afford only IX. The mechanistic implications in reference to the di-π-methane process of V are discussed.
IT **82639-36-9**
RL: PRP (Properties)
(photolysis and thermolysis of, biradicals in)
RN 82639-36-9 HCAPLUS
CN 3,8[1',2']-Benzenoindeno[2,1-c]pyrazole, 3,3a,8,8a-tetrahydro- (9CI) (CA INDEX NAME)

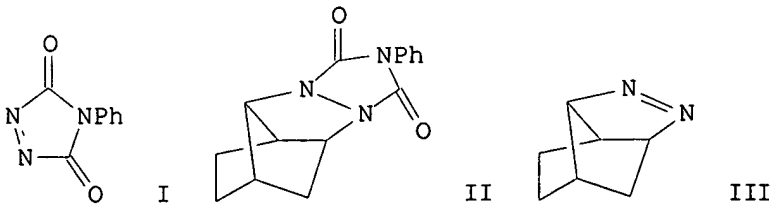


IT **82639-37-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion to polycyclic azaalkane)
RN 82639-37-0 HCAPLUS
CN 5,10[1',2']-Benzeno-1H-indeno[2',1':3,4]pyrazolo[1,2-a][1,2,4]triazole-1,3(2H)-dione, 4a,5,9b,10-tetrahydro-2-methyl- (9CI) (CA INDEX NAME)



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)

L3 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1980:471653 HCAPLUS
DOCUMENT NUMBER: 93:71653
ORIGINAL REFERENCE NO.: 93:11653a,11656a
TITLE: Bicyclic azoalkanes via urazoles derived from cycloaddition of N-phenyl-1,2,4-triazoline-3,5-dione with strained bicycloalkenes
AUTHOR(S): Adam, Waldemar; De Lucchi, Ottorino; Erden, Ihsan
CORPORATE SOURCE: Dep. Chem., Univ. Puerto Rico, Rio Piedras, 00931, P. R.
SOURCE: Journal of the American Chemical Society (1980), 102(14), 4806-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 93:71653
GI



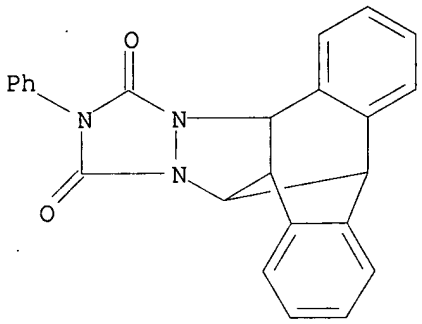
I II III

AB Cycloaddn. of the triazoline I to strained bicycloalkenes leads to urazoles, e.g. II, via skeletal rearrangement of dipolar intermediates. This novel reaction appears to be general, including benzoannelated, spiroannelated, alkylidene-functionalized, and heteroatom-substituted substrates. Bicyclo[2.2.2]octene is not sufficiently strained to undergo reaction with I. Ene reaction and homo-Diels-Alder addition will suppress this useful dipolar I cycloaddn. Oxidation hydrolysis of the urazoles provides a convenient entry into the hitherto unknown polycyclic azoalkanes, e.g., III, possessing C-type skeletons.

IT **73818-05-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and spectra of)

RN 73818-05-0 HCAPLUS

CN 5,10[1',2']-Benzeno-1H-indeno[2',1':3,4]pyrazolo[1,2-a][1,2,4]triazole-1,3(2H)-dione, 4a,5,9b,10-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)

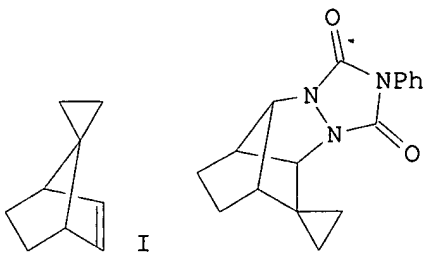


OS.CITING REF COUNT: 13 THERE ARE 13 CAPLUS RECORDS THAT CITE THIS RECORD (13 CITINGS)

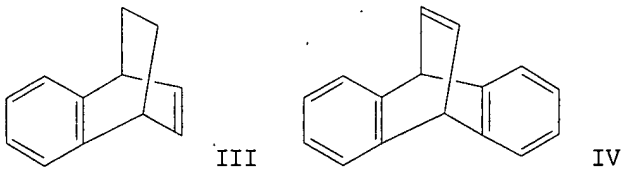
L3 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER:	1980:408091 HCAPLUS
DOCUMENT NUMBER:	93:8091
ORIGINAL REFERENCE NO.:	93:1483a,1486a
TITLE:	Cycloaddition of 4-phenyl-1,2,4-triazoline-3,5-dione (PTAD) to bicycloalkenes via rearrangement of zwitterionic intermediates
AUTHOR(S):	Adam, Waldemar; De Lucchi, Ottorino
CORPORATE SOURCE:	Dep. Chem., Univ. Puerto Rico, Rio Piedras, 00931, P. R.
SOURCE:	Tetrahedron Letters (1979), (45), 4367-70 CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE:	Journal
LANGUAGE:	English

GI



I II



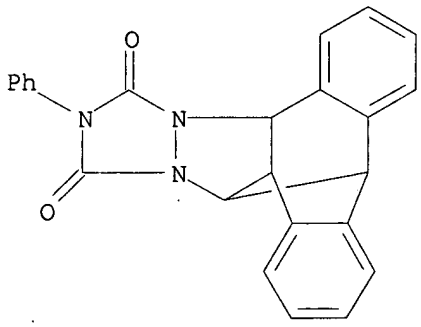
III IV

AB PTAD reacted with functionalized, moderately strained, and benzoannulated bicyclic olefins to give tricyclic urazoles through rearrangement of intermediary 1,4-dipoles. E.g., alkene I with PTAD at reflux gave 70% of the urazole II. Alkenes III and IV gave 17 and 63%, resp., of the corresponding urazoles.

IT **73818-05-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 73818-05-0 HCAPLUS

CN 5,10[1',2']-Benzeno-1H-indeno[2',1':3,4]pyrazolo[1,2-a][1,2,4]triazole-1,3(2H)-dione, 4a,5,9b,10-tetrahydro-2-phenyl- (9CI) (CA INDEX NAME)



L3 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1979:121387 HCAPLUS

DOCUMENT NUMBER: 90:121387

ORIGINAL REFERENCE NO.: 90:19214h,19215a

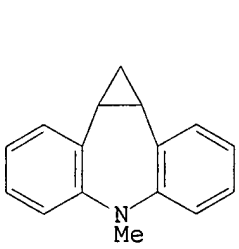
TITLE: Synthesis of dibenzo[b,f]cycloprop[d]azepine derivatives. III. Introduction of a cyclopropane ring by thermal decomposition of a pyrazoline

AUTHOR(S): Kawashima, Kenya; Kawano, Yasuhiko

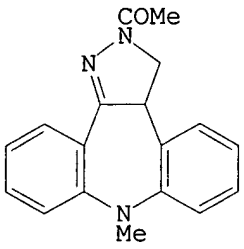
CORPORATE SOURCE: Takeda Res. Lab., Takeda Chem. Ind., Ltd., Osaka, Japan

SOURCE: Takeda Kenkyushoho (1978), 37(1-2), 6-11
CODEN: TAKHAA; ISSN: 0371-5167

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 90:121387
GI



I

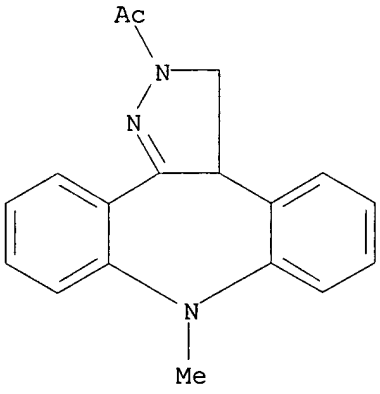


II

AB The title compound, I was prepared by thermal decomposition of the pyrazoloazepine
II. Pyrolysis of II, prepared from 5-methyl-5H-dibenz[b,f]azepine or 5,11-dihydro-5-methyl-10H-dibenz[b,f]azepin-10-one, at 200° in an evacuated system in the presence of NaOH gave I in 49.3% yield.

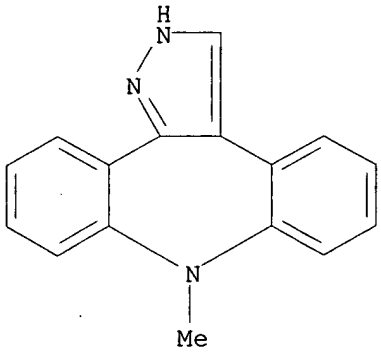
IT **55397-02-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermal decomposition of, methyldibenzocyclopropazepine from)

RN 55397-02-9 HCAPLUS
CN Ethanone, 1-(3a,8-dihydro-8-methyldibenzo[b,f]pyrazolo[4,3-d]azepin-2(3H)-yl)- (CA INDEX NAME)

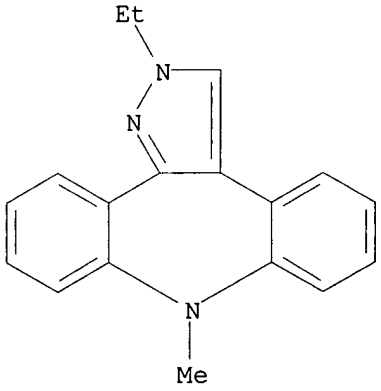


IT **69512-34-1P 69512-35-2P 69512-36-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

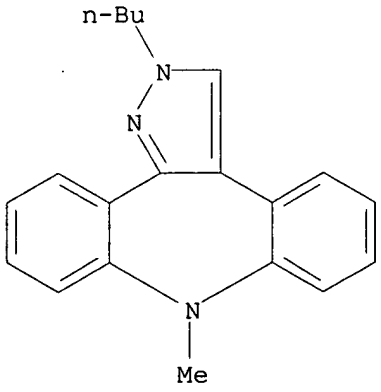
RN 69512-34-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine, 2,8-dihydro-8-methyl- (CA INDEX NAME)



RN 69512-35-2 HCAPLUS
CN Dibenzo[b,f]pyrazolo[4,3-d]azepine, 2-ethyl-2,8-dihydro-8-methyl- (CA INDEX NAME)



RN 69512-36-3 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 2-butyl-2,8-dihydro-8-methyl- (CA INDEX NAME)

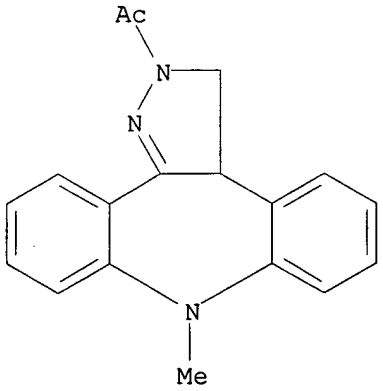


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)

L3 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1975:156133 HCAPLUS
DOCUMENT NUMBER: 82:156133
ORIGINAL REFERENCE NO.: 82:24913a,24916a
TITLE: 1,1a,6,10b-Tetrahydro-6-alkyldibenzo[b,f]cycloprop[d]azepines
INVENTOR(S): Kawashima, Kenya; Kawano, Yasuhiko
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49100093	A	19740920	JP 1973-13934	19730202
PRIORITY APPLN. INFO.:			JP 1973-13934 A	19730202

GI For diagram(s), see printed CA Issue.
AB Azepines I (R = lower alkyl) are prepared by heating dibenzo[b,f]pyrazolo[3,4-d]azepines II (R1 = lower alkyl) in the presence of alkali. Thus, heating III (R2 = H) with paraformaldehyde-Me2NH.HCl in EtOH gave III (R2 = CH2NMe2), which was refluxed with N2H4 in AcOH to give II (R = R1 = Me), which was heated with NaOH at 200° for 24 hr in a sealed tube to give I (R = Me).
IT **55397-02-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring contraction of)
RN 55397-02-9 HCAPLUS
CN Ethanone, 1-(3a,8-dihydro-8-methyldibenzo[b,f]pyrazolo[4,3-d]azepin-2(3H)-yl)- (CA INDEX NAME)



L3 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1962:436315 HCAPLUS
DOCUMENT NUMBER: 57:36315
ORIGINAL REFERENCE NO.: 57:7246d-i,7247a-i,7248a-i,7249a-i,7250a-c
TITLE: 1,3-Dipolar addition. I. Diphenylnitrilimine and its 1,3-dipolar additions to alkenes and alkynes

AUTHOR(S): Huisgen, Rolf; Seidel, Michael; Wallbillich, Guenter; Knupfer, Hans
CORPORATE SOURCE: Univ. Munich, Germany
SOURCE: Tetrahedron (1962), 17, 3-29
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: German

AB The previously undescribed diphenylnitrilimine PhCNNPh (I) is available by elimination of N from 2,5-diphenyltetrazole (II) at 160° or by dehydrochlorination of PhCCl:NNHPh (III) at 20-80° with NEt3. I adds in situ to alkenes and alkynes forming 1,3-diphenyl-Δ2 pyrazolines and 1,3-diphenylpyrazoles, resp. PhNHNHBz (40 g.) and 48 g. PCl3 refluxed 10 hrs. (H2O-free atmospheric) in 50 ml. anhydrous Et2O and the clear solution treated with 80 g. PhOH in 60 ml. Et2O and with 80 ml. MeOH, the main part of the Et2O evaporated with rise of internal temperature to 60-70°, and the cooled mixture filtered yielded 58% III, m. 129.530.5°. III (460 mg.) and 0.50 g. norbornene in 4 ml. anhydrous C6H6 treated at 20° with 1.0 ml. NEt3 and the mixture kept several hrs., filtered from Et3NHCl, m. 253-5°, and the filtrate and washings evaporated yielded 85% bicyclo[2.2.1]hept-2-ene adduct, 1,3-diphenyl-4,7-methano-3a,4,5,6,7,7ahexahydroindazole (IV), m. 171-2° (alc.), λ 244, 370 mμ (log ε 4.14, 4.32), strongly blue-green fluorescent in daylight, brown-yellow color in concentrated H2SO4 turning dark green in addition of concentrated HNO3. III (500 mg.) and 0.50 g. norbornene in 5 ml. C6H6 shaken 8 hrs. with 200 mg. KOH in 1.5 ml. H2O at 20° yielded 76% IV, also produced in 94% yield by treating III and norbornene in boiling C6H6 with Et3N. IV in CHCl3 treated with 1.0 mole-equivalent Br (exothermic reaction) and the cooled mixture washed with KOH and H2O, evaporated, and the residue sublimed at 120-40°/ 0.003 mm. gave 1-(p-bromophenyl-3-phenyl-4,7-methano3a,4,5,6,7,7a-hexahydroindazole, m. 133-4° (alc.), ν 800, 825 cm.-1 II (2.0 g.) in 10 ml. dicyclopentadiene (V) heated 3 hrs. at 160-5° with liberation of 9.0 millimoles N and the unchanged V distilled at 10 mm. yielded 68% 1,3-diphenyl4,8-methano-3a,4,4a,7,8,8a - hexahydroindeno [5,6-c] pyrazole (VI), m. 173-4°. III (460 mg.) and 1.2 g. V in 6 ml. C6H6 refluxed 1 hr. with addition of 1.0 ml. Et3N and the filtered solution evaporated yielded 87% VI, λ 242, 370 mμ (log 4.15, 4.33, CHCl3). VI (3.0 g.) refluxed 42 hrs. with 3.0 g. chloranil in 20 ml. xylene and the dark brown solution extracted repeatedly with 4% KOH, the H2O-washed solution freed from solvent and distilled at 120-65°/0.003 mm., the glassy product crystallized from 60 ml. hot alc., and the crystalline material (0.90 g.) sublimed in vacuo gave non-fluorescent 1,3-diphenyl4,8 - methano - 4,4a,7a,8 - tetrahydroindeno[5,6 - c]pyrazole (VII), m. 124.0-4.5°. VI (653 mg.) heated 3 hrs. at 200-55° with 90 mg. S with evolution of H2S and the product sublimed at 120-70°/0.01 mm. yielded 48% 1,3-diphenylpyrazole, m. 84-5° (petr. ether). III (460 mg.) and 2.25 g. bicycloheptadiene in 7 ml. C6H6 heated 3 hrs. at 65° with 1.0 ml. Et3N and kept 16 hrs. at 20°, the mixture filtered from 1.97 millimoles Et3NHCl and the filtrate evaporated, the residue boiled in 50 ml. alc. and filtered from 27 mg. insol. product, the solution cooled, and the crystalline material (79%) recrystd. from ligroine (b. 80-120°) yielded 1,3-diphenyl4,7-methano-3a,4,7,7a-tetrahydroindazole (VIII), m. 133-5° (decomposition), λ 243, 369 mμ (log ε 4.13, 4.30). The insol. product recovered from HCONMe3 gave bright greenish yellow amorphous 1,3,5,7-tetraphenyl-4,8-methano-3a,4,-

4a,7a,8,8a-hexahydropyrazolo[4,5-f]indazole, m. above 320° (decomposition), λ 244, 359, mμ (log ε 4.39, 4.52). VIII (2.29 g.) heated slowly from 130 to 185° several min. with vigorous evolution of gas through a trap at -78°, condensing 77% cyclopentadiene (identified as maleic anhydride adduct, m. 165.0-5.5°), and the residue distilled at 135-50°/0.003 mm. yielded 98% 1,3-diphenylpyrazole. III (2.00 millimoles) and 4.0 millimoles endo-cis-bicyclo[2.2.1]hept-5-ene-2,3dicarboxylic acid anhydride refluxed 1 hr. in 4 ml. C6H6 with dropwise addition of 1.0 ml. Et3N in 2 ml. C6H6 and the mixture refluxed 1 hr., filtered from Et3NHCl, and the residue on evaporation recrystd. from EtOAc gave 55% pale green 1,3diphenyl-4,7-methano-3a,4,5,6,7,7a-hexahydroindazole-5,6dicarboxylic acid anhydride, m. 279-81° (decomposition). The dipolarophilic activity of normal unconjugated double bonds is relatively small as shown by a comparative study of the addition of I to non-conjugated alkenes, diphenylketene, and ketene acetal. III (3.98 millimoles), 21.5 millimoles C5HnCH:CH2, and 1.5 ml. Et3N heated 30 hrs. at 80-90° in a sealed tube and the filtered solution evaporated, the residue distilled at 160-80°/0.001 mm. and the yellow oil crystallized from MeOH yielded 85% 1,3-diphenyl-5-pentyl-Δ2-pyrazoline, m. 56-8° (MeOH), dehydrated (0.75 millimole) by refluxing 2 hrs. with 1.5 millimoles chloranil in 25 ml. xylene, the pale yellow oily 1,3-diphenyl-5-pentylpyrazole oxidized 80 min. in boiling 50% C6H5N with 2 g. KMnO4, washed with Et2O and filtered from MnO2, treated with Na2SO3 and acidified to yield 0.13 g. 1,3-diphenyl-5-pyrazolecarboxylic acid (IX), m. 225-60° (H2O). Ill (3.98 millimoles) similarly treated with 16.5 millimoles H2C:CH(CH2)8CO2Et and the product distilled at 200-30°/0.003 mm. gave 80% material, recrystd. from MeOH to yield yellow needles of Et 9-(1,3-diphenyl-Δ2-pyrazolin-5-yl)nonanecarboxylate, m. 40-2°. III with 3 mole-equivs. unsatd. ester in boiling C6H6 and the product distilled yielded also 28% tetraphenyldihydrotetrazine, m. 200-3°, produced by head-to-tail dimerization of I and showing the lacking activity of the dipolarophile. III (1.99 millimoles), 11.3 millimoles cyclopentene and Et3N refluxed 150 min. in 5 ml. C6H6 and the mixture kept 16 hrs., the residue on evaporation of the filtrate sublimed in a high vacuum, and the sublimate recrystd. from alc. yielded 78% 1,3-diphenyl-cis-1,3a,4,5,6,6a-hexahydrocyclopentapyrazole (X), m. 137.5-9.0°, λ 241,365 mμ (log ε 4.12, 4.31, CHCl3), with blue-green fluorescence. III (2.00 millimoles), 0.7 g. Ph2C:CO refluxed with Et3N in C6H6 and the filtered solution evaporated, the residue distilled at 150-220°/0.001 mm. and the red oil (1.06 g.) recrystd from alc. gave 0.19 g. 1,3,4,4-tetraphenyl-Δ2-pyrazol-5-one, m. 160-2°, ν 1712 cm.-1 III (2.00 millimoles) and 7.6 millimoles H2C:C(OEt)2 refluxed with Et3N in C6H6 without separation of Et3NHCl, the filtered solution evaporated, the residue distilled at 160-70°/0.004 mm., the red oil (0.50 g.) chromatographed in C6H6 over Al2O3 (Merck, activity I), and the eluate crystallized from 90% alc. gave 0.42 g. 1,3-diphenyl-5-ethoxypyrazole, m. 67-9°, λ 275 mμ (log ε 4.36). The pyrazole (0.53 g.) refluxed 9 days in 5 ml. alc. and 7 ml. concentrated HCl, the cooled mixture neutralized with NaOH and extracted with CH2Cl2, the product distilled in a high vacuum, and the distillate recrystd. from alc. and ligroine (b. 80-110°) yielded 75% 1,3-diphenyl-Δ2-pyrazol-5-one, m. 136.0-7.5°, 1708 cm.-1 The orientation in the addition of I to Ph2C:CO and to H2C:C(OEt)2 is that to be expected in regarding PhC+: N-N-Ph as a representation of I. III (2.31 g.) and 2.5 1. butadiene in 40 ml. C6H6

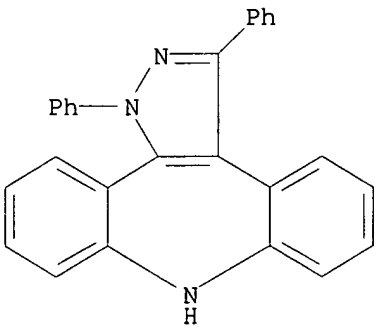
shaken 4 hrs. with 3 ml. Et3N under pressure and kept several days, the blue fluorescent mixture filtered, and the residue on evaporation recrystd. from alc. gave 2.34 g. crystalline 1,3-diphenyl-5-vinyl-Δ2-pyrazoline (XI), m. 76.0-7.5°, b0.001 130-40°. XI (4.0 millimoles) refluxed 10 hrs. with 4.7 millimoles chloranil in 10 ml. xylene and filtered from 2.9 millimoles tetrachlorohydroquinone, the filtrate extracted with alkali, and the washed solution evaporated gave 0.87 g. noncryst. viscous oil, distilled at 158-80°/0.001 mm. The oil (0.61 g.) in 45 ml. Me2CO stirred 2 hrs. with gradual addition of 1.25 g. KMnO4 and kept 30 min. before reduction with SO2 and extraction with CH2Cl2, the residue on evaporation crystallized from CCl4 and MeOH, and the product (0.41 g.), m. 227.08.5° (decomposition), recrystd. gave IX. PhCH:CHCOCH2CO2Et and PhNHNH2 gave the known Et 1,3-diphenyl-5-methyl-4-pyrazolinecarboxylate (XII), dehydrogenated with chloranil in xylene to Et 1,3-diphenyl-5-methyl-4-pyrazolecarboxylate and saponified by alkali and decarboxylated to 1,3-diphenyl-5-methylpyrazole, m. 46-7° (Et2O-petr. ether), refluxed (2.0 g.) 2 hrs. with 6 g. KMnO4 in 100 ml. 1:1 stabilized Me2CO-H2O, the filtered solution acidified with 2N HCl, and the product recrystd. from MeOH gave 31% starting material and 24% IX, m. 228-9° (decomposition), neutralization equivalent 261. III (1.99 millimoles) and 3.0 millimoles cyclopentadiene kept 20 hrs. with NEt3 in C6H6 and the product purified by crystallization from alc. and sublimation in a high vacuum gave 0.30 g. 1,3-diphenyl-cis-1,3a,4,6a-tetrahydrocyclopentapyrazole, m. 183-4°, λ 242, 367 mμ (log ε 4.11, 4.31, CHCl3), oxidized with KMnO4 in Me2CO at 20° to give 1,3-diphenyl-4-pyrazolecarboxylic acid and BzOH, brominated with 1.0 molar equivalent Br in C6H6 to 1-(4-bromophenyl)-3-phenyl-cis-1,3a,4,6a-tetrahydrocyclopentapyrazole, m. 148-50° (alc.), ν 820 cm.-1 and hydrogenated (300 mg.) in 80 ml. EtOAc at 20° in 50 min. with Raney Ni to give 0.29 g.X. III treated with 5 molar equivs. cyclohexa-1,3-diene in C6H6 in the presence of Et3N yielded 73% 1,3-diphenyl-3a,4,5,7a-tetrahydro-indazole, b0.005 150-60°, m. 119.5-21.0° (alc.), dehydrogen ated with chloranil in boiling xylene 18 hrs., the product distilled in a high vacuum and crystallized from MeOH yielded 79% 1,3-diphenylindazole, m. 100.5-2.0°. III (1.99 millimoles) and 0.91 g. freshly distilled styrene kept 2 hrs. at 60° with Et3N and some hydroquinone in C6H6 and the product recrystd, from MeOH yielded 88% 1,3,5-triphenyl-Δ2pyrazoline, m. 137-8°, λ 240, 361 mμ (log ε 4.20, 4.28). II (2.0 g.) heated 3 hrs. at 155-65° in 5 ml. 1,2-dihydronaphthalene with loss of 0.98 molar equivalent N, the excess d dihydronaphthalene evapd, i@ vacuo, and the residue crystallized from MeOH yielded 2.44 g. material, m. 133-48°. Treatment of 3.5 molar equivs. dihydronaphthalene with III in C6H6 in the presence of NEt3 yielded 75% product, recrystd. 4 times from alc. to give 1,3-diphenyl-3a,4,5,9b-tetrahydronaphtho[1,2-c]pyrazole, m. 151-2°, dehydrogenated with chloranil in C6H3Cl3 52 hrs. at 170°, the product distilled in a high vacuum and triturated with petr. ether yielded 70% 1,3-diphenylnaphtho[1,2-c]pyrazole (XIII), m. 100.5-2.0° (petr. ether, alc.). PhNHNH2 (1.2 ml.) and 2.48 g. 2,1BzC10H6OH heated (N atmospheric) 16 hrs. at 150° in 5 ml. EtOCH2CH2OH containing 20 mg. p-MeC6H4SO3H, the mixture stirred into H2O and the red-brown product recrystd. from alc. yielded 72% phenyl 1-hydroxy-2-naphthyl ketone phenylhydrazone (XIV), b0.001 220-30°, m. 130.0-1.5°. XI (1.02 g.) kept 2 hrs. at 95° in 70 ml. polyphosphone acid and the solution poured into 200 ml. ice H2O, the yellow precipitate distilled at 210-30°/0.001 mm., and the

distillate chromatographed from C6H6 on Al2O3 (Woelm, acid, activity I) gave 0.56 g. XIII. Treatment of 117 with 3.5 mole-equivs. indene in C6H6 in the presence of NEt3 and the product sublimed at 140-70°/0.004 ml. gave 482 mg. 1,3-diphenyl-3a,8b-dihydro-4H-indeno[1,2-c]pyrazole, m. 171-2°, λ 239, 364 mμ (log ε 4.15, 4.28).
Similarly 2.8 mole-equivs. transstilbene in C6H6 yielded 86% 1,3,4,5tetraphenyl-4,5-trans-dihydropyrazole, m. 166.5-8.0°(alc.), refluxed 50 hrs. in xylene with chloranil, the dehydrogenation product distilled in vacuo and recrystd. from C6H12 gave 1,3,4,5-tetraphenylpyrazole (XV), m. 217-19°. III (4.0 millimoles) heated 3 days at 50° with 3.6 g. cisstilbene in a sealed tube and the adduct (53%) crystallized from CH2Cl2alc. gave greenish yellow needles of 1,3,4,5-tetraphenyl 4,5-cis-dihydropyrazole, m. 194.5-5.5°, taken up (110 mg.) in 5 ml. boiling Me2CO and treated gradually with 60 mg. KMnO4 in 20 ml. Me2CO, reduced with SO2, and the Me2CO evaporated to give 108 mg. XV. III (2.0 millimoles) in C6H6 treated with 6.0 millimoles acenaphthylene in the presence of Et3N 1 hr. at 80° and 7 hrs. at 20°, filtered from Et3N-HCl, and the product (90%) recrystd. from PhMe gave 7,9diphenyl - 6b,9a - dihydroacenaphtho[1,2 - c] pyrazole, m. 255.5-7.5° (decomposition). Dibenzo[b,f]azepine (1.20 g.) refluxed 2.5 hrs. in 10 ml. C6H6 with 1.43 g. III and 4.3 ml. NEt3 and the precipitate washed free from NEt3HCl with H2O yielded 55% material, recrystd. repeatedly from xylene to give 1,3-diphenyldibenzo [b,f] pyrazolo [3,4-d] azepiue, m. 264.0-5.5°, λ 302, 361 mμ (log ε 4.07, 4.14), ν 3335 cm.-1 Ill treated by the usual procedure with 3 mole-equivs. H2C:CHCO2Et 45 min. at 20% gave 85% Et 1,3-diphenylΔ2-pyrazoline-5-carboxylate, m. 99-101° (MeOH), dehydrogenated with chloranil in boiling xylene to yield 94% Et 1,3-diphenyl-5-pyrazolecarboxylate, m. 84.5-6.0°, hydrolyzed with KOH in MeOH to IX. Similar reaction with 7 mole-equivs. H2C:CHCN 30 min. at 20° yielded 85% 1,3-diphenyl-5-cyano-Δ2-pyrazoline, m. 138-40°, aromatized by refluxing 2 hrs. in xylene with chloranil to give 76% 1,3-diphenyl-5-cyanopyrazole, m. 133-5°, ν 2240 cm.-1, hydrolyzed by 2 hrs. reflux in 1:1:1 H2SO4-AcOH-H2O to yield IX. II (2.0 g.) heated 8 hrs. at 155-65° in 7 ml. PhCH:CHCO2Et with liberation of 97% N, the excess ester evaporated, and the residue crystallized from alc. yielded 2.86 g. isomeric mixture, m. 113-16°. The mixture (2.0 g.) refluxed 20 hrs. in 10 ml. xylene with 5.7 millimoles chloranil and the product, m. 127-33°, recrystd. twice from alc. yielded 50% Et 1,3,5-triphenyl-4-pyrazolecarboxylate, m. 142-5°. Treatment of HI with 2 mole-equivs. PhCH:CHCO2Et in boiling C6H6 with NEt3 yielded 83% isomeric mixture, m. 116-23°. The direction of the addition seemed to be influenced more strongly by steric than by electronic factors. II (1.0 g.) heated 2 hrs. at 160-70° in 5 ml. MeCOCH2CO2Et with evolution of 104% N and the residue distilled at 170-80°/ 0.01 mm. yielded 67% rapidly solidifying oil, recrystd. from C6H12-Et2O to give XII, also obtained in 19% yield by thermolysis of II in EtOCH:CHCO2Et, and in 62% yield by decomposition of II in AcOCH:CHCO2Et. Hydrolysis of XII with 12% KOH in MeOH gave 1,3-diphenyl-5-methyl-4pyrazolecarboxylic acid, m. 193-4° (alc.). II (9.0 millimoles) and 6 g. maleic anhydride heated 5 hrs. in 20 ml. MeOPh at 155° and the product recrystd. from C6H6 gave 1.21 g. 1,3-diphenyl-Δ2-pyrazoline-cis-4,5-dicarboxylic anhydride (XVI), m. 191)-2° (decomposition) (determination made in preheated bath at 180°). Decomposition of II at 160-70° caused decomposition of XVI in 3 hrs. with formation of 35% 1,3-diphenylpyrazolc. II (9.0 millimoles) heated in 5 g. trans-MeO2CCH:CHCO2Me with evolution of 0.94 moleequiv. N yielded 88% di-Me 1,3-diphcnyl-Δ2-pyrazolinetrans-4,5-dicarboxylate (XVII), m. 148-50° (alc.), also prepared in 99% yield by treatment with III in C6H6 with NEt3. XVI taken up in hot aqueous Na2CO3

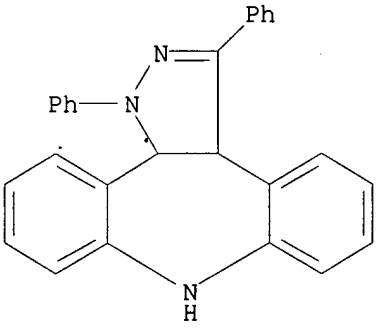
and the dicarboxylic acid esterified with CH2N2 gave XVII. XVII (1.5 g.) refluxed 20 hrs. in xylene with 6.1 millimoles chloranil and the product crystallized from alc. gave 1.17 g. di-Me 1,3-diphenylpyrazole-4,5-dicarboxylate (XVIII), m. 151.2°. II (9.0 millimoles) in 5 g. cis-MeO2CCH:CHCO2Me heated, the excess ester distilled, and the residue fractionated from alc. yielded 51% XVII and 4% di-Mc 1,3-dil)henyl-Δ2-pyrazolinecis-4,5-dicarboxylate, m. 141-3°, also produced in 72% yield by keeping XVI 3 days in dilute Me2CO and esterifying the product with CH2N2. II (9.0 millimoles) refluxed 6 hrs. in 20 ml. MeOPh containing 5.0) g. di-Mc malcic anhydride with evolution of 255 ml. N, the solvent and excess dipolarophile distilled, and the residue extracted with Et2O gave 1.58 g. residue, recrystd. repeatedly from C6H12 to give 1,3diphenyl-4,5-dimethyl-Δ2-pyrazoline-cis-4,5-dicarboxylic anhydride, m. 138-4°. III (3.98 millimoles), 2.9 g. trans-MeO2CMe:CMeCO2Me, and 1.5 ml. NEt3 heated 2 days at 50° in a sealed tube and the product crystallized from MeOH yielded 74% di-Me 1,3-diphenyl-4,5-dimethyl-Δ2-pyrazoline- trans-4,5-dicarboxylate, m. 107.5-8.5°. Similarly III and 5 mole-equivs. cis-MeO2CCMe:CMeCO2Me gave 33% di-Me 1,3-diphenyl-4,5-dimethyl-Δ2-pyrazoline-cis-4,5-dicarboxylate, m. 144-5°, also obtained from the cis-anhydride in 67% yield. II (9.0 millimoles) and 3 g. α-naphthoquinone heated 2 hrs. at 160-70°, the residue digested with Et2O and crystallized from CHCl3 yielded 85% 1,3-diphenyl-4,9-dioxo-4,9-dihydronaphtho[2,3-c]pyrazole, m. 257-9°. II (2.25 millimoles) refluxed 3 hrs. in 5 ml. MeOPh with 0.6 g. 2-methyl-α-naphthoquinone gave 0.27 g. 1,3-diphenyl-9a-methyl- 4,9 - dioxo-33,4,9,9a-tetrahydronaphtho[2,3-c]pyrazole, m. 245-7° (CHCl3), ν 1780 cm.-1 The reciprocal action of I with the CC triple bond led directly to aromatic pyrazole systems. III (1.30 millimoles) in 3 ml. PhC:CH heated on a steam bath with dropwise addition of 1.0 ml. NEt3, kept 1.5 hrs., the cooled mixture filtered from 95% Et3NHCl, the filtrate distilled at 130-50°/0.003 mm., the red oil chromatographed on basic Al2O3, eluted with C6H6, and the middle fraction recrystd. from MeOH yielded 72% 1,3,5-triphenylpyrazole (XVIII), m. 138.5-9.5°. II (9.0 millimoles) heated 6 hrs. at 155-65° with PhC:CPh with liberation of 235 ml. N gave 34% XIV, obtained only in 2.6% yield by treatment with III in C6H6 in the presence of Et3N. II (9.0 millimoles) heated in 5 ml. HC:CCH(OPr)2 and the product distilled at 190-205°/0.001 mm. gave 2.82 g. oily 1,3-diphenylpyrazole-5-aldehyde dipropyl acetal, hydrolyzed 48 hrs. at 20° in 20 ml. dioxane and 10 ml. 50% HCl to yield 79% 1,3-diphenyl-5-pyrazolecarboxaldehyde, m. 138-40°; 2,4-dinitrophenylhydrazone m. 260° (dccompn.). The aldehyde refluxed 2 hrs. in MeOCH2CH2OH with moist Ag2O and the neutral and acidic products gave 35% IX. III with 2.5 mole-equivs. HC:CCO2Me gave 71% Me 1,3-diphenyl-5-pyrazolecarboxylate, m. 111.512.5° (MeOH), hydrolyzed quant. with KOH in MeOH to IX.

II (5.4 millimoles) decomposed in 4 g. PhC:CCO2Et yielded 84% di-Et 1,3,5-triphenyl-4-pyrazolecarboxylate, m. 144-5° (alc.), saponified with KOH in MeOH to 90% 1,3,5-triphenyl-4-pyrazolecarboxylic acid, m. 239-41° (decomposition) decarboxylated at 245° to XVIII. II (9.0 millimoles) and 5 ml. Me2O2CC:CCO2Me heated and the product distilled at 210-30°/0.001 mm. yielded 56% di-Me 1,3-diphenylpyrazole-4,5-dicarboxylate, m. 153-4°, saponified to the dicarboxylic acid, m. 198-200° (decomposition), neutralization equivalent 170, decarboxylated by heating 30 min. at 200° to give 1,3-diphenylpyrazole-4-carboxylic acid, m. 201-3°, neutralization equivalent 270°. Proof of cis addition and determination of the orientation rules represent contributions to the mechanism of 1,3-dipolar addition

IT **85008-87-3P**
RL: SPN (Synthetic preparation); PRP (Properties); PREP (Preparation)
(1,3-Dipolar addition. I. Diphenylnitrilimine and its 1,3-dipolar additions to alkenes and alkynes)
RN 85008-87-3 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,8-dihydro-1,3-diphenyl- (CA INDEX NAME)



IT **85008-85-1P**, Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl-
RL: PREP (Preparation)
(preparation of)
RN 85008-85-1 HCAPLUS
CN Dibenzo[b,f]pyrazolo[3,4-d]azepine, 1,3a,8,12b-tetrahydro-1,3-diphenyl- (CA INDEX NAME)



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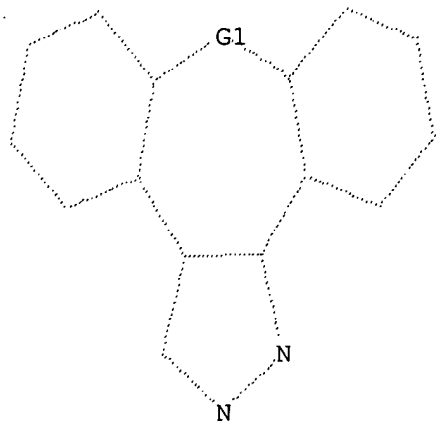

G1 C,S,N

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Structure attributes must be viewed using STN Express query preparation.
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L3            16 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2
L5             1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3 AND CNS


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                 DIS
L2            94 SEA SSS FUL L1

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L3            16 SEA ABB=ON  PLU=ON  L2
L4             1 SEA ABB=ON  PLU=ON  L3 AND NEUROTRANSMITTER
L5             1 SEA ABB=ON  PLU=ON  L3 AND CNS
                 D L3 IBIB ABS HITSTR 1-16
                 D QUE STAT


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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Aug 2009

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